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-> b reg
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STRUCTURE FILE UPDATES:   27 JAN 2008  HIGHEST RN 1000849-38-6
DICTIONARY FILE UPDATES:  27 JAN 2008  HIGHEST RN 1000849-38-6

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predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

-> d que sta l9
L5                STR

Hy~Hy~G1
 1   2   3


VAR G1=AK/CB
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT  IS E6 C  E1 N  AT   1
ECOUNT  IS E4 C  E2 N  AT   2

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L7          3902 SEA FILE=REGISTRY ABB=ON  PLU=ON  NCNC3/ES AND NC6/ES
L9           301 SEA FILE=REGISTRY SUB=L7 SSS FUL L5

100.0% PROCESSED    3902 ITERATIONS                          301 ANSWERS
SEARCH TIME: 00.00.01



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L7          3902 SEA FILE=REGISTRY ABB=ON  PLU=ON  NCNC3/ES AND NC6/ES
L25               STR

Hy~Hy==N
 1   2   3


NODE ATTRIBUTES:
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DEFAULT ECLEVEL IS LIMITED
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ECOUNT  IS E4 C  E2 N  AT   2

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
L27         2294 SEA FILE=REGISTRY SUB=L7 SSS FUL L25

100.0% PROCESSED    3902 ITERATIONS                         2294 ANSWERS
SEARCH TIME: 00.00.01
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FILE 'HCAPLUS' ENTERED AT 18:04:10 ON 28 JAN 2008
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FILE COVERS 1907 - 28 Jan 2008  VOL 148 ISS 5
FILE LAST UPDATED: 27 Jan 2008  (20080127/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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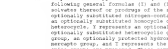
L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:515480 HCAPLUS
DN 141:71535
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 inhibitors
IN Watanabe, Tatsuki; Nishiko, Masaya; Shibayama, Shiro; Toda, Hideaki; Ito, Kazuhiro
PA Sai Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 442 pp.
DESIGN PATENT
LI Kokai
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004052862	A2	20040624	WO2003-JP15714	20031209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU2003304794	A1	20040630	AU2003-304794	20031209
EP---1571148	A1	20050907	EP2003-778753	20031209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US2007047459	A1	20070719	2005US-539758	20050610
PRAI JP2002-356146	A	20021206		
JP2003-142734	A	20030520		
JP2003-251710	W	20031209		
OS MARPAT 141:71535				

GI



AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted benzene ring or a nitrogen-containing heterocycle, Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group, and Y represents the ring A or an optionally substituted heterocyclic group) are disclosed. The compds. are CXCR4 inhibitors, particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cancerous tumor, cancer metastasis, rheumatoid arthritis, osteoporosis, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR5 receptors on CD4-pos. cells. All the compds. prepd. in Examples 1-1 to 1-3 showed inhibitory activity of ≥1381[nmol SDF-] to CEM cells, more specifically 3.3 μM for N-(1-benzylpyrrolidin-3-ylmethyl)-4-(pentyloxypyridin-3-yl)pyrimidine. An aspirin and tablet formulation containing 2-((5-(dimethylaminomethyl)amino)-4-(pentyloxypyridin-3-yl)pyrimidine were described.

IT 71990-44-6P 71990-45-7P 71990-46-8P
71990-47-9P 71990-48-0P 71990-49-1P
71990-50-4P 71990-51-5P 71990-52-6P

L12 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
71990-39-9P 71991-26-2P 71991-73-9P
71991-74-0P
RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(preps. of nitrogen-containing heterocyclic compds. as CXCR4 antagonists for prophylaxis and/or treatment of diseases)
IT 71990-44-6P
RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(preparation of nitrogen-containing heterocyclic compds. as CXCR4 antagonists for prophylaxis and/or treatment of diseases)
RN 71990-44-6 HCAPLUS
CN 1,2-Ethanediamine, N'-[[5-(hexyloxy)-3-pyridinyl]-5-(trifluoromethyl)-4-pyrimidinyl]-N,N-dimethyl-, (9CI) (CA INDEX NAME)

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=> d bib abs hitstr 135 tot
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L31 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2004:515487 HCAPLUS
DN 141:7155
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 inhibitors
IN Watanabe, Tatsuo; Sokoto, Masaya; Shibayama, Shiro; Toda, Hideaki; Ito, Kazuhiro
PA Sai Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 441 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004057983	A2	20040715	WO 2003-JP15974	20031209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AM, CH, CN, DE, DK, EA, EP, ES, FI, FR, GB, GH, GM, GR, HU, IE, IT, KE, LS, LU, MC, MW, MZ, NL, OA, PT, RO, SD, SE, SI, SK, SL, SZ, TR, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2003303674	A1	20040727	AU 2003-303674	20031209
EP 1571148	A1	20050907	EP 2003-778753	20031209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 20070167459	A1	20070719	US 2005-538758	20050610
PRAI JP 2002-358748	A	20021210		
JP 2003134436	A	20030509		
JP 2003-415718	A	20031209		
WO 2003-JP15974	W	20031209		

GI

AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted benzene or heterocycle; the ring C represents a heterocycle, Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group, and Y represents the ring A or an optionally substituted hydrocarbyl group) are disclosed. These compds. are CXCR4 receptor antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cancer, tumor metastasis, osteoporosis, rheumatism, diabetes, cancer, and aspects for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the exemplified compds. showed IC50 values of 1 μM or less for binding of (125I)human SDF-1 to CEM cells, more specifically 0.3 μM for N-(1-benzylpyrrolidin-3-ylmethyl)-4-(pentyltetrahydropyran-4-ylmethyl)amino]-4-piperidinecarboxamide. An example and tablet formulation containing 2-[(5-dimethylaminomethyl)amino]-4-(pentyltetrahydropyran-4-yl)pyrimidine were described.

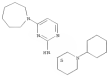
IT 713098-41-2P 713098-44-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

L31 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(Uses)
(prepn. of nitrogen-containg heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)
RN 713098-41-2 HCAPLUS
CN 2-Pyrimidinamine, N-[(3S)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-2H-pyran-4-yl)- (CA INDEX NAME)

Absolute stereochemistry.

RN 713098-44-5 HCAPLUS
CN 2-Pyrimidinamine, N-[(3S)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-4-yl)- (CA INDEX NAME)

Absolute stereochemistry.



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L14 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 2002:614505 HCAPLUS
DN 137:165235
TI Preparation of anxiolytic pyrrolidinones as NOS inhibitors
IN Atwal, Kamaljit S.; Bedley, Glen J.; Dorsey, David S.; Durbin, Johnes J.; Hoover, Raymond R.; Kowalczyk, Brian A.; Lovering, Frank E.; Rovnyak, George C.; Shapiro, Michael J.; Stringer, Richard A.; Swanson, Richard N.; Tozzo, Estelle; Vaidyanathan Haridas, Parthasarathy, Jr.; Phillips, Gary B.; Yu, Kai; Zhou, Jianhua
PA Bristol-Myers Squibb Co., USA; Pharmacopeia, Inc.
SO U.S. 131 pp., Cont'-in-part of U.S. Ser. No. 10,124, abandoned.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 3

PATENT NO	KIND	DATE	APPLICATION NO.	DATE
PI US--6410744	A1	20020813	1999US-1139213	19990826 <--
CA--2126777	B	20030105	1993CA-2126777	19980219 <--
AT--343339	T	20061215	1998AT-2906455	19980219 <--
EP--1754703	A2	20070221	2006EP-0023849	19980219 <--
EP--1754703	A3	20070328		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE, MC, PT, SE, SK				
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CA--2178255	A1	20010301	2001CA-2178255	20000814 <--
WO2001014414	A1	20010301	2000WO-US22284	20000814 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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US2002148050	A1	20021017	2002US-0103598	20020402 <--
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L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN (Continued)

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	US----6846847	B2	20050308		
	EP----1351683	A1	20031022	2002EP-0706933	20020523 <--
PRAI	1997US-0908975	B2	19970730		
	1998US-0031215	A3	19980223	<--
	1998US-0039178	A	19980313	<--
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	1999US-0303613	A	19990504	<--
	2000WO-US23173	W	20000814	<--
OS	MARPAT 137:165234			
GI				

AB The title compds. [I; R = H, CH3 (R5 = H, halo, alkyl, optionally substituted alkyl or cycloalkyl); R1 = H, halo, alkyl, optionally substituted alkyl, alkyl, aralkyl, cycloalkyl; R4 = H, CH3; X, Y, Z = N, CR13 (R13 = H, alkyl, cycloprop(yl, halo, haloalkyl); A = H3, OR2, COOR12, SO(NR12)2, SO2(OR12, etc. (R2, R12 = H, optionally substituted alkyl or cycloalkyl, etc.; NR1R2 = N-heterocyclyl); B = CH2)(CHR14)nNR2R3 (n = 1-4; R3 = H, alkyl, cycloalkyl, optionally substituted alkyl, aryl, etc.; R2 = H, alkyl; Q = CH2, CO, SO2, C(:NR15), C(:NR16)(:CR17); R14 = H, halo, alkyl; R15 = H, alkyl; or R = C = halo; R14, R16 = H, alkyl; n = 1-3), useful as inhibitors of nitric oxide synthase, were prepared [thus, N-((1,3-benzodioxol-5-yl)methyl)-3-(1H-imidazol-1-yl)phenylpiperidine-3-carboxamide was prepared by reaction of 3-(3-aminophenyl)aldehyde, 4(3-chloro-2-methoxybenzoate, and piperonylamine. All exemplified compds. (
IT 212562-02-3P 212562-03-4P 212562-04-5P
212562-05-6P 212562-06-7P 212562-07-8P
212562-08-9P 212562-09-0P 212562-10-3P
212562-11-4P 212562-12-5P 212562-13-6P
212562-14-7P 212562-15-8P 212562-16-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation), USES (Uses)
(preparation of imidazolyl pyrrolidinamines as NOS inhibitors)
RN 212562-02-3 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[(1H-imidazol-1-yl)-4-methyl-4-pyridinyl]- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 212562-03-4 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-(2-(3,3-dihydro-1,4-benzodioxin-6-yl)ethyl)hexahydro-1-[(1H-imidazol-1-yl)-4-methyl-4-pyridinyl]- (CA INDEX NAME)

RN 212562-04-5 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]hexahydro-1-[5-(1H-imidazol-1-yl)-4-methyl-4-pyridinyl]- (CA INDEX NAME)

RN 212562-11-4 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[5-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-4-methyl-4-pyridinyl]- (CA INDEX NAME)

RN 212562-16-9 HCAPLUS
CN 1H-Azepine-2-carboxamide, N-[2-(3,4-diethoxyphenyl)ethyl]-1-[4-ethyl-1-(1H-imidazol-1-yl)-4-pyridinyl]hexahydro- (CA INDEX NAME)

L18 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 312650-33-0 HCAPLUS
CN L8-Acyclae-2-carboxamide, N-[3,4-dimethoxybenzyl]methyl]hexahydro-1-[2-[18-imidazol-1-yl]-4-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

RN 312650-35-2 HCAPLUS
CN L8-Acyclae-2-acetamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-[18-imidazol-1-yl]-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

RN 312650-36-3 HCAPLUS
CN L8-Acyclae-2-acetamide, N-(3,5-dimethoxybenzyl)hexahydro-1-[6-ethyl-2-[18-imidazol-1-yl]-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

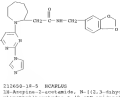
L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 312650-21-0 HCAPLUS
CN L8-Acyclae-2-acetamide, N-[2-[3,4-dimethoxyphenyl]ethyl]hexahydro-1-[2-[18-imidazol-1-yl]-4-methyl-4-pyrimidinyl]- (CA INDEX NAME)

RN 312650-22-1 HCAPLUS
CN L8-Acyclae-2-acetamide, N-[3-[3,4-dimethoxyphenyl]ethyl]hexahydro-1-[2-[18-imidazol-1-yl]-4-[1-methylethyl]-4-pyrimidinyl]- (CA INDEX NAME)

RN 312650-24-3 HCAPLUS
CN L8-Acyclae-2-acetamide, hexahydro-1-[2-[18-imidazol-1-yl]-4-methyl-4-pyrimidinyl]-N-[(4-methoxyphenyl)methyl]- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 312650-1F-5 HCAPLUS
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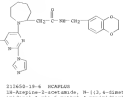
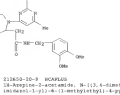
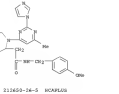


RN 312650-1H-6 HCAPLUS
CN L8-Acepine-2-acetamide, N-[(2,4-dimethoxyphenyl)methyl]hexahydro-1-[2-[18-imidazol-1-yl]-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

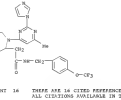


RN 312650-20-9 HCAPLUS
CN L8-Acepine-2-acetamide, N-[(2,4-dimethoxyphenyl)methyl]hexahydro-1-[2-[18-imidazol-1-yl]-4-(3-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

L19 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 312650-24-5 HCAPLUS
CN L8-Acepine-2-acetamide, hexahydro-1-[2-[18-imidazol-1-yl]-6-methyl-4-pyrimidinyl]-N-[[4-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)



RE.CNT 1A THERE ARE 1A CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

AN 1998:604917 HCAPLUS

DN 129:231019

TI Preparation of N-heterocyclic derivatives as NOS inhibitors

IN Arnaiz, Damian O.; Baldwin, John J.; Davey, David D.; Devlin, James J.; Dolle, Roland Ellwood, III; Erickson, Shawn David; McMillan, Kirk; Morrissey, Michael M.; Ohlmeyer, Hichael H. J.; Pan, Gonghua; Paradkar, Vidyadhar Madhav; Parkinson, John; Phillips, Gary B.; Ye, Bin; Zhao, Zuchun; et al

PA Berlex Laboratories, Inc., USA; Pharmacopeia, Inc.; et al.

SO PCT Int. Appl., 358 pp.
CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 3

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO---9837079	A1	19980827	1998WO-US03176	19980219	<--
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	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, GM, GA, GN, ML, MR, NE, SN, TD, TG					
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	CA---2281545	C	20070424			
	AU---9861749	A	19980909	1998AU-0061749	19980219	<--
	AU----732969	B2	20010503			
	EP----968206	A1	20000105	1998EP-0906555	19980219	<--
	EP----968206	B1	20061115			
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	NZ----337861	A	20010223	1998NZ-0337861	19980219	<--
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	HU2002004228	A3	20030528			
	RU---2241708	C2	20041210	1999RU-0120077	19980219	<--
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	EP---1754703	A3	20070228			
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	NO----321664	B1	20060619			
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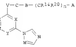
	US2003027794	A1	20030206	2002US-0121758	20020412	<--
	US---6846829	B2	20050125			
	US2003060452	A1	20030327	2002US-0121212	20020412	<--
	US---6849739	B2	20050201			
	US2003069210	A1	20030410	2002US-0122072	20020412	<--
	US---6841674	B2	20050111			
PRAI	1997US-0808975	A2	19970219	<--		
	1998US-0025124	A	19980217	<--		
	1998EP-0906555	A3	19980219	<--		
	1998WO-US03176	W	19980219	<--		
	1999US-0383813	A3	19990826	<--		

OS MARPAT 129:231019

GI



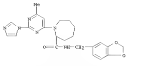
I

AB N-Heterocyclic derivs. I [U = N, CR5 (R5 = H, halo, alkyl, optionally substituted aralkyl or aryl, etc.), V = NR4, S, O, CHR4 (R4 = H, alkyl, aryl, aralkyl, cycloalkyl), W = N, CH; X, Y, Z = N, CR19 (R19 = H, alkyl, cyclopropyl, halo, haloalkyl); A = R1, OR1, CONR1R2, PO(NR1R2)2, NR1COR2, etc. (R1, R2 = H, optionally substituted alkyl or cycloalkyl, etc. or R1R2N = N-heterocyclyl); B = CR17(CHR15)mQR3 (m = 1-4, R3 = H, alkyl, cycloalkyl, optionally substituted aryl, etc.; R15, R17 = H, alkyl; Q = CO, O, C:NR1, etc.), N-heterocyclyl; C = (CHR12)q(CHR13)r (q, r = 0 or 1; R12, R13 = H, alkyl); or B = C = null; R14, R20 = H, alkyl, n = 1-3] were prepared as inhibitors of nitric oxide synthase. Thus, N-[(1,3-benzodioxol-5-yl)methyl]-1-[3-(1H-imidazol-1-yl)phenyl]piperidine-2-acetamide was prepared by reaction of 1-(3-aminophenyl)imidazole, 7-chloro-3-oxoheptanoic acid Et ester, and piperonylamine.

IT 212650-00-5P 212650-01-6P 212650-03-8P
212650-05-0P 212650-06-1P 212650-09-4P
212650-11-8P 212650-12-9P 212650-13-0P
212650-15-2P 212650-16-3P 212650-18-5P
212650-19-6P 212650-20-9P 212650-21-0P
212650-22-1P 212650-24-3P 212650-26-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-heterocyclic derivs. as NOS inhibitors)

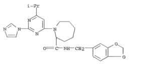
RN 212650-00-5 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



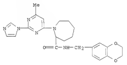
RN 212650-01-6 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



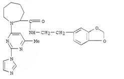
RN 212650-03-8 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[(2,3-dihydro-1,4-benzodioxin-6-yl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



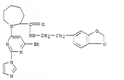
RN 212650-05-0 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



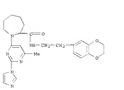
RN 212650-06-1 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[2-(1,3-benzodioxol-5-yl)ethyl]-1-[6-ethyl-2-(1H-imidazol-1-yl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



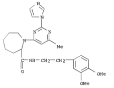
RN 212650-09-4 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[2-(2,3-dihydro-1,4-benzodioxin-6-yl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



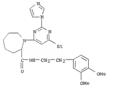
RN 212650-11-8 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



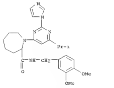
RN 212650-12-9 HCAPLUS

CN 1H-Azepine-2-carboxamide, N-[2-(3,4-dimethoxyphenyl)ethyl]-1-[6-ethyl-2-(1H-imidazol-1-yl)-4-pyrimidinyl]hexahydro- (CA INDEX NAME)



RN 212650-13-0 HCAPLUS

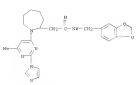
CN 1H-Azepine-2-carboxamide, N-[(3,4-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



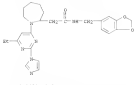
RN 212650-15-2 HCAPLUS

CN 1H-Azepine-2-acetamide, N-(1,3-benzodioxol-5-ylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

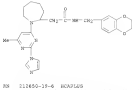
L14 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-16-3 HCAPLUS
CN 1H-Azepine-2-acetamide, N-(2,3-benzofuranyl-5-ylmethyl)-1-(6-ethyl-2-(1H-imidazol-1-yl)-4-pyrimidinyl)hexahydro- (CA INDEX NAME)

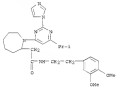


RN 212650-18-5 HCAPLUS
CN 1H-Azepine-2-acetamide, N-(2,3-dihydro-1,4-benzodioxin-6-ylmethyl)hexahydro-1-[6-(1H-imidazol-1-yl)-4-methyl-4-pyrimidinyl]- (CA INDEX NAME)

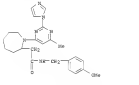


RN 212650-19-6 HCAPLUS
CN 1H-Azepine-2-acetamide, N-(3,4-dimethoxyphenylmethyl)hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)

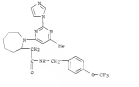
L19 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-24-3 HCAPLUS
CN 1H-Azepine-2-acetamide, hexahydro-1-[5-[(4-imidazol-1-yl)-6-methyl-4-pyrimidinyl]-4H-[4-methoxyphenyl]methyl]- (CA INDEX NAME)

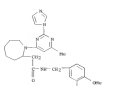


RN 212650-26-5 HCAPLUS
CN 1H-Azepine-2-acetamide, hexahydro-1-[5-[(4-imidazol-1-yl)-6-methyl-4-pyrimidinyl]-4H-[4-(trifluoromethoxy)phenyl]methyl]- (CA INDEX NAME)

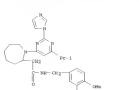


RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD.
ALL CITATIONS AVAILABLE IN THE RE FORMAT

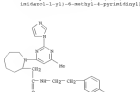
L19 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 212650-20-9 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[(2,6-dimethoxyphenyl)methyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(1-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-21-0 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-methyl-4-pyrimidinyl]- (CA INDEX NAME)



RN 212650-22-1 HCAPLUS
CN 1H-Azepine-2-acetamide, N-[2-(3,4-dimethoxyphenyl)ethyl]hexahydro-1-[2-(1H-imidazol-1-yl)-6-(3-methylethyl)-4-pyrimidinyl]- (CA INDEX NAME)

L19 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:478163 HCAPLUS
DN 85:78163
ORGREF 85:12564a
TI 4-Ketos-4-aroylpyrimidines and salts useful for relaxation of smooth muscle in a mammal
IN De Angelis, Gerald G.; Benz, Hans J. E.
PA Pfizer Inc., USA
SO U.S., Division of U.S. 3,959,112.
CODEN: XBXXAM
DT Patent
LA English
FAN.CNT 4

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI US---3950255	A	1976Apr13	1975US-0567306	1975Apr11	<--
US---3959112	A	1976May25	1975US-0582210	1975Jun03	<--
US---3959112	A	1976?05	1973US-0371683	1973Jun19	<--
PRAI 1973US-0371683	A3	1973Jun19	<--		
1972US-0272443	A3	1972Jul19	<--		
1975US-0578216	A2	1975May06	<--		
1975US-0578216	A2	1975May06	<--		

GI

AB Pyrimidinones I (R = Ph, substituted phenyl, furyl, thienyl, naphthyl; R1 and R2 = H, alkyl, hydroxyalkyl, aminoalkyl; NR1R2 = heterocyclic; R3 = H, Me, Et, Pr, CHMe2) (100 compds.) were prepared and have platelet aggregation-inhibiting and bronchodilator properties. Thus, I (R = Ph, R1 = R2 = Et, R3 = H) were obtained by Grignard reaction of PhMe with NCCH2CO2Et, condensation of NCHCPh(CH2CO2Et) with HCONMe2, chlorination of the resulting 4-hydroxypyrimidine, and amination of the 4-chloro compound
IT 3441-21-0P
RL: RPH (Pharmaceutical preparation), PREP (Preparation)
(preparation of)
RN 3441-21-0 HCAPLUS
CN 1H-Azepine-2-acetic acid, hexahydro-1-(4-phenyl-6-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L14 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1996:59510 HCAPLUS
DN 64:59518
ORGREF 64:9803a,9804a
TI Arylpyrimidines, inhibitors of platelet aggregation and bronchodilators
IN De Angelis, Gerald G.; Hess, Hans J. E.
PA Pfizer Inc.
SO U.S., 27 pp. Division of U.S. 3,450,699.
CODEN: XIXXAM
DT Patent
LA English
FAN.CNT 1

PI	US----3518017	A	19700623	19730619 <--
	US----3717640	A	19731206	19700605 <--
	US----3717641	A	19731206	19700605 <--
	DE----23057	A	19720210	19730216 <--
	US----3893221	A	19750617	19730619 <--
	CA----878243	A3	19751015	19730619 <--
	CA----978532	A2	19751125	19740128 <--
	US----3857844	A	19741231	19731101 <--
	FI----49844	B	19780630	
PRAI	1970US-0012166	A2	19700216 <--	
	1970US-0083218	A3	19710930 <--	
	1971FI-0002734	A	19711930 <--	
	1971US-0116711	A3	19710216 <--	
	1973CA-0214322	A3	19731024 <--	

TI For diagram(s), see printed CA issue.
AB About 140 pyrimidines [R = H, 2-ClC6H4, 2-furyl, 2-thienyl, 3-HOC6H4, etc.; R1 = H, Me; R2, R3 = H(CH), NaSH, Bu2N, 1-pyrrolidinyl, 4-morpholinyl, 4-methyl-1-piperazinyl, PhCH2NH, etc.] creating chloroacetic/diaryloxyacetic anilides followed by cleavage, thio-, HOCH2CH2Br was treated with PhNgBr and the HONCPh(CH2)2Br cyclized with NaOMeEt to give 1 (R = Ph, R1 = H, R2 = OH), which was chlorinated with PSCl3 and treated with EtOCHN to give 2 (R = Ph, R1 = H, R2 = Et2N). At 10-4 g/l (R = Ph, R1 = H, R2 = Et2N) inhibited in vitro platelet aggregations by 99%. At 40 mg/kg (R = 3-HOC6H4, R1 = H, R2 = Et2N) showed bronchodilation against histamine induced bronchoconstriction in guinea pigs.
IT 36422-43-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platelet aggregation inhibition of)
RN 36422-43-9 HCAPLUS
CN 1H-Azepine, hexahydro-1-(4-phenyl-4-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L19 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:173049 HCAPLUS
DN 82:173049
ORGREF 82:2734a,2734b
TI 4-Pyrimidinylcholinesterase oxide
IN Pearson, Claude; Eberle, Jeremiah; Boergary, Guy; Surwood, Guy; Gouret, Jacques
PA Specialede S. A., Fr
SO Fr. Demande, 13 pp. Addn to Fr. 2,154,081 (Occ Cor. 2,252,822. CA 79,92896x)
CODEN: FRXXBL
DT Patent
LA French
FAN.CNT 1

PI	FR----2225154	A1	19741108	1973FR-0013967	19730416 <--
	FR----2225154	A2	19790701		
PRAI	1973FR-0013967	A	19730416 <--		

TI For diagram(s), see printed CA issue.
AB Analgesic and antiinflammatory (no data) pyrimidinylmorpholydromic acids [R = H, Me; R1 = H, alkyl, cycloalkyl, alkenyl, alkynyl, aralkyl, morpholinyl; R2 = NHCH2, R3 = 3-ClC6H4, 3,4,5-(MeO)3C6H2; 3-ClC6H4, 3,4-methylenedioxyphenyl] were prepared by treating 1 (R2 = OEt) with NHCH2R1.
IT 41556-49-6P 42556-79-8P 59675-39-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41556-49-6 HCAPLUS
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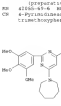
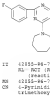


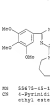
RN 42556-79-8 HCAPLUS
CN 4-Pyrimidinecarboxamide, 6-(hexahydro-1H-azepin-1-yl)-N-hydroxy-2-(3-trifluoromethylphenyl)- (CA INDEX NAME)

RN 59675-39-3 HCAPLUS
CN 4-Pyrimidinecarboxamide, 2-(3-fluorophenyl)-6-(hexahydro-1H-azepin-1-yl)-N-hydroxy- (CA INDEX NAME)

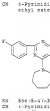
L19 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



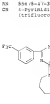
IT 42556-86-7 59675-42-1 59675-47-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of, with hydroxylamine)
RN 42556-86-7 HCAPLUS
CN 4-Pyrimidinecarboxylic acid, 6-(hexahydro-1H-azepin-1-yl)-2-(3,4,5-trimethoxyphenyl)-, ethyl ester (CA INDEX NAME)



RN 59675-43-1 HCAPLUS
CN 4-Pyrimidinecarboxylic acid, 2-(3-fluorophenyl)-6-(hexahydro-1H-azepin-1-yl)-, ethyl ester (CA INDEX NAME)



RN 936 8-13-3 HCAPLUS
CN 5-Hydrolinecarbol acte, 4-(hexahydro-1H-azepin-1-yl)-2-(3-(trifluoromethyl)phenyl)-, ethyl ester (CA INDEX NAME)



L19 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1971:64806 HCAPLUS
DN 77:64806
ORGREF 77:9934a
TI 4-Arylpyrimidines for inhibiting thromboxyte aggregation and as bronchodilators
IN De Angelis, Gerald G.; Hess, Hans J. E.
PA Pfizer Inc.
SO U.S., 27 pp.
CODEN: USXXAM
DT Patent
LA German
FAN.CNT 2

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	1971NL-0004901	A	19710601 <--		
	1973ES-0410209	A3	19731202 <--		

GI For diagram(s), see printed CA issue.
AB 4-Halo-6-arylpyrimidines (I, useful for inhibition of thromboxyte aggregation and as bronchodilators, were prepared by reaction of 90g2 with H2N(CH2)nCH2X to give AcC(NH2)2CH2CONR1, which was condensed with RCO2R2 to give the 4-hydroxy analog of I, treated with PSCl3, and PCl2NR. Other methods included reaction of substituted 4-chlorobenzotrile with H2N(CH2)nCH2X to give ClC6H4C(NH)NH(CH2)nCH2X, which was condensed with RCONH2 to give a 4-hydroxy-1-(hexahydroazepin)2,5-diphyridine-treatment with PSCl3, PCl2NR, then H over Pd/C, or by condensation of RCH2NHCH2CHOR with (NH2)2CO to give a 4-aryl-5-acetoxypyrimidine which was hydrogenated over Pd/C, treated with PSCl3, then PCl2NR. Thus, 2-(3-ClC6H4)-4-OH-6-(hexahydro-1H-azepin-1-yl)pyrimidine (II; R1, R2 = H, Cl-4 alkyl, alkyl; R3 = H, Cl-4 alkyl, CF3CH2, alkyl, R4,R5(CH2)2, 2-pyridyl; or R3R4 = (CH2)4-6, (CH2)2N(CH2)2, or

L18 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(CH2)2NH+(CH2)2) were prepd.
IT 868620-81-9P
RL: RCT (Reactant or reagent); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of pyrimidinylpiperidine derivs. as histamine H3 receptor ligands)
RN 868620-81-9 HCAPLUS
CN 1H-Azepine, hexahydro-3-(6-phenyl-4-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

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=> d bib abs hitind hitstr 140 tot
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L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:796691 HCAPLUS
DN 139:307788
TI Preparation of 5-cyanopyrimidine derivatives as anti-inflammatory agents
IN Machii, Daisuke; Yamaura, Yosuke; Arai, Hitoshi; Yanagawa, Koji; Ohshima, Etsuo; Kawanabe, Ari; Iwase, Miho; Kobayashi, Katsuya; Sato, Takashi; Miki, Ichiro
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003082855	A1	20031009	2003WO-JP04009	20030328
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OS MARPAT 139:307788
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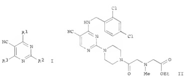
I II

AB The title pyrimidine compds. I [wherein R1 and R3 = independently H, OH, halo, (un)substituted alkyl, alkoxy, alkylthio, aryl, aralkyl, or amino; R2 = (un)substituted amino] or ammonium salts or pharmaceutically acceptable salts thereof are prepared as anti-inflammatory agents. For example, the compound II was prepared in a multi-step synthesis. II showed 97% inhibitory activity against thymus and activation-regulated chemokine (TARC) Hut78 cells at 1 μM. Formulations containing I as an active ingredient were also described.
IC ICM C07D-401/12
ICS C07D-239/42; C07D-401/04; C07D-405/12; C07D-413/04; C07D-401/14; C07D-403/12; C07D-403/04; A61K-031/506; A61K-031/5377; A61K-031/541; A61K-031/55; A61P-029/00; A61P-037/08; A61P-043/00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
IT Chemokines
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(thymus and activation-regulated, macrophage-derived; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
IT 611199-85-0P 611199-86-1P 611199-87-2P 611199-88-3P 611199-89-4P
611199-90-7P 611199-91-8P 611199-92-9P 611199-93-0P 611199-94-1P

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
RN 611200-40-9 HCAPLUS
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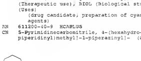

RN 611200-41-0 HCAPLUS
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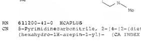
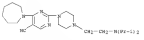


RN 611200-42-1 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[4-[2-[bis(1-methylethyl)amino]ethyl]-1-piperazinyl]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

L40 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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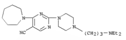
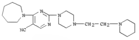


RN 611200-44-3 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-(hexahydro-1H-azepin-1-yl)-2-[4-[2-(1-piperidinyl)ethyl]-1-piperazinyl]- (CA INDEX NAME)



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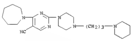

RN 611201-14-0 HCAPLUS
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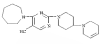
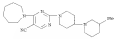
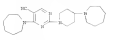


RN 611201-15-1 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-(hexahydro-1H-azepin-1-yl)-2-(3-methyl[1,4'-bipiperidin]-1'-yl)- (CA INDEX NAME)



RN 611201-26-2 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-(hexahydro-1H-azepin-1-yl)-2-[4-(hexahydro-1H-azepin-1-yl)-1-piperidinyl]- (CA INDEX NAME)



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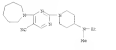
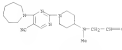


RN 611201-38-4 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-(hexahydro-1H-azepin-1-yl)-2-[4-(methyl-2-propynylamino)-1-piperidinyl]-, (9CI) (CA INDEX NAME)



RN 611202-14-3 HCAPLUS
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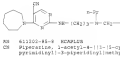
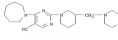
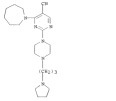


RN 611202-84-9 HCAPLUS
CN Piperazine, 1-acetyl-4-[[1-[5-cyano-4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]-3-piperidinyl]methyl]- (9CI) (CA INDEX NAME)



RN 611204-90-9 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-(hexahydro-1H-azepin-1-yl)-2-[4-[3-[1-pyrrolidinyl]propyl]-1-piperazinyl]- (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L2             TRA L1 1- RN :     1829 TERMS

     FILE 'REGISTRY' ENTERED AT 17:03:07 ON 28 JAN 2008
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L4          1375 L3 AND NC6/ES AND  46.195.39/RID
L5                STR
L6             0 L5
L7          3902 NCNC3/ES AND NC6/ES
L8             7 L5 SAM SUB=L7
L9           301 L5 FULL SUB=L7
                 SAV TEM J758C1/A L9
L10           13 L9 AND L3

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     FILE 'REGISTRY' ENTERED AT 17:11:22 ON 28 JAN 2008
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L14           61 L13 AND (PD<=20031209 OR AD<=20031209 OR PRD<=20031209)
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L20            0 L17

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                 E E3+ALL
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                 E E22+ALL
L22        27324 E10+OLD,NT
L23            2 L21-22 AND L13
                 SEL HIT RN 2
                 SEL AN 2 L23
L24            1 E15-16 AND L23

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L29          926 L27 NOT L28
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L37            32 L36 AND (PD<=20031209 OR AD<=20031209 OR PRD<=20031209)
L38             2 L37 AND L21-22
L39             1 L23 NOT L38
L40             1 L24 AND L27

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STRUCTURE FILE UPDATES:   18 FEB 2008  HIGHEST RN 1004360-55-7
DICTIONARY FILE UPDATES:  18 FEB 2008  HIGHEST RN 1004360-55-7

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=> d que sta l9
L5              STR

Hy~^Hy~^N
1   2   3


NODE ATTRIBUTES:
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ECOUNT  IS E6 C  E1 N  AT   1
ECOUNT  IS E4 C  E2 N  AT   2

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   3

STEREO ATTRIBUTES: NONE
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L9          2301 SEA FILE=REGISTRY SUB=L7 SSS FUL L5

100.0% PROCESSED    3911 ITERATIONS                          2301 ANSWERS
SEARCH TIME: 00.00.01


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FILE COVERS 1907 - 19 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008 (20080218/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d bib abs hitstr l22 1

L13 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2006:363486 HCAPLUS
DN 144:429480
TI Method for measuring cell migration activity
IN Shibuya-ma, Shinji, Sakada, Satsuhiko, Watanabe, Noriki, Sugiyama, Tetsuya
PA Ono Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO	DATE
PI WO2006042804	A1	20060427	2005WO-JP19187	20051019

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRAI JP2004-302429 20041018

AB A method is provided for measuring the cell migration activity corresponding to the function of a specific cell migration inducer in vivo. The method comprises: (1) a process for transferring cells producing a cell migration inducer (e.g., MSX, SDF-1) into an air-pouch formed in the back subcutis of a mammal; (2) a process for recovering the transferring cells to be measured (e.g., T cells, B cells, monocytes, macrophages, granulocytes) into a site other than the air-pouch of the mammal; (3) a process for recovering the cells in the air-pouch; and (4) a process for measuring the number of the cells to be measured in the recovered cells. Also provided are a method for evaluating a cell migration inhibitory component possessing a specificity or a selectivity in vivo using the above method and a method for producing the above cell migration inhibitory component.

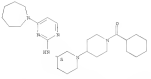
IT 718981-91-4

RL: BSU (Biological study, unclassified); BIOL (Biological study)
(method for measuring cell migration activity)

RN 718981-91-4

CN [1,4'-Bipiperidin]-3-amine, 1'-(cyclohexylmethoxy)-N-[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry



RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d bib abs hitrn fhitstr l22 2
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L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 2004:515487 HCAPLUS

DN 141:71555

TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 regulators

IN Habashita, Hiromu; Kokubo, Masaya; Shibayama, Shiro; Tada, Hideaki; Tanihiro, Tatsuya

PA Ono Pharmaceutical Co., Ltd., Japan

SO PCT Int. Appl., 641 pp.
CODEN: PIXXD2

DT Patent

LA Japanese

FAN.CNT 1

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	RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	EP---1571146	A1	20050907	2003EP-0778753	20031209
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	US2007167459	A1	20070719	2005US-0538758	20050610
PRAI	2002JP-0357446	A	20021210		
	2003JP-0162706	A	20030606		
	2003WO-JP15718	W	20031209		

OS MARPAT 141:71555

GI

 I

 II

AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted homocycle or an optionally substituted heterocycle, Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group, and T represents the ring A or an optionally substituted amino group) are prepared. These compds. are CXCR4 regulators, in particular CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cerebral diseases, cardiovascular diseases, metabolic diseases, or cancer, and agents for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the compds. prepared showed IC50 of 10 μM for inhibiting the binding of [125I]human SDF-1 to CEM cells, more specifically 0.1 μM for 2-(1-benzylpyrrolidin-3-ylamino)-4-(perhydroazepin-1-yl)pyrimidine. An ampule and tablet formulation containing 2-[[2-(dimethylamino)ethyl]amino]-4-(perhydroazepin-1-yl)pyrimidine were described.

IT 710978-26-0P 710978-30-6P 710978-41-9P
710978-46-4P 710978-49-7P 710978-55-5P
710978-59-9P 710978-64-6P 710978-70-4P

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

710978-75-9P 710979-06-9P 710979-13-8P
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710989-50-7P 710989-53-0P 710989-56-3P

L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

710989-59-6P 710989-62-1P 710989-65-4P
710989-68-7P 710989-71-2P 710989-74-5P
710989-77-8P 710989-80-3P 710989-85-8P
710989-88-1P 710989-90-5P 710989-93-8P
710989-96-1P 710989-99-4P 710990-01-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 710990-03-7P 710990-06-0P 710990-08-2P
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710990-54-8P 710990-56-0P 710990-59-3P
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L22 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

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710993-43-4P 710993-44-5P 710993-45-6P
710993-46-7P 710993-47-8P 710993-49-0P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 710993-56-9P 710993-58-1P 710993-60-5P
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710996-41-1P 710996-42-2P 710996-43-3P

RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 710996-44-4P 710996-45-5P 710996-46-6P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study); PREP (Preparation), USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 711001-19-3P 711001-20-6P 711001-27-3P
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711004-78-3P 711004-79-4P 711004-80-7P
711004-81-8P 711004-82-9P 711004-83-0P
711004-84-1P 711004-85-2P 711004-86-3P
711004-87-4P 711004-88-5P 711004-89-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use), BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg. heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 711004-90-9P 711004-91-0P 711004-92-1P
711004-93-2P 711004-94-3P 711004-95-4P
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713138-10-4P 713138-11-5P 713138-12-6P
713138-13-7P 713138-14-8P 713138-15-9P
713138-16-0P 713138-17-1P 713138-18-2P
713138-19-3P 713138-20-6P 713138-21-7P
713138-22-8P 713138-23-9P

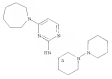
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use), BIOL (Biological study), PREP (Preparation); USES (Uses)
(prepn. of nitrogen-contg heterocyclic compds. as CXCR4 antagonists for prepn. and/treatment of diseases)

IT 711002-73-2P
RL: RCT (Reactant), SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heterocyclic compds as CXCR4 antagonists for preparation and/treatment of diseases)

IT 710978-26-0P
RL: PAC (Pharmacological activity), SPN (Synthetic preparation), THU (Therapeutic use), BIOL (Biological study), PREP (Preparation), USES (Uses)
(preparation of nitrogen-containing heterocyclic compds as CXCR4 antagonists for preparation and/treatment of diseases)

RN 710978-26-0 HCAPLUS
CN 2-Pyrimidinamine, N-(3S)-[1,1'-bipiperidin]-3-yl-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

Absolute stereochemistry



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L11 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 2004:46 6603 HCAPLUS
DN 141:38617
TI Preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol (pi) 3-kinase inhibitors and their use in the treatment of cancer
IN Hunt, John T.; Mitt, Dennis; Rathnow, Paul A.
PA Bristol-Myers Squibb Co., USA
SO PCT Int. Appl., 144 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004043965	A1	20040610	WO2003-US37284	20031121 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
CA 2517102	A1	20040610	2003CA-2517102	20031121 <--
AU 2003294	A1	20040618	2003AU-0294	20031121
US 2004116	A1	20040617	2003US-0719896	20031121
EP 1567	A1	20050831	2003EP-0786982	20031121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
BR 2003087	A	20050927	2003BR-0087	20031121
CN 1	A	20060111	CN 2003-80108139	20031121
JP 2006514	T	20060427	2005JP-0510083	20031121
MX 2005006	A	20050725	2005MX-0006477	20050613
CA 2509	A	20060927	2005CA-2509615	20050608
NO 2005	A	20050708	2005NO-2003017	20050615
ZA 2005	A	20060329	2005ZA-0004913	20050615
PRAI 2002US-0427198	P	20021121		
2003US-0719896	P	20031107		
2003US-0730219	P	20031119		
2003WO-US37284	W	20031121		

OS MARPAT 141:38617
GI

I

II

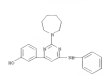
L11 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

AB Title compds: I [X = (un)substituted alkyl(ene/yn)i, hetero/aryl, heteroaryl(alkyl); R = H, alkenyl, alkynyl, and cert. CHO and derivs.; R1 = (un)substituted alkyl, cycloalkyl, heterocyclyl, or NR2 and derivs.; R2 = (un)substituted alkyl, cycloalkyl, heterocyclyl, or NR3 and derivs.; (un)substituted alkyl, cyclyl containing at least one heteroatom, with provisos, their stereoisomers, tautomers, pharmaceutically acceptable salts, esters, or prodrugs] were prepared as phosphatidylinositol (pi) 3-kinase inhibitors for treating neoplasm. A solid phase synthesis is described in which the resin-bound selected I displayed an IC50 < 1 uM in a cell proliferation assay.

IT 781263-14-3P, 3-[2-(Azepan-1-yl)-4-(1H-indazol-5-yl)amino]pyrimidin-6-yl]phenol
RL: SPN (Synthetic preparation); PUR (Purification or recovery); PREP (Preparation)
(preparation of 2,4,6-trisubstituted pyrimidines as phosphatidylinositol 3-kinase inhibitors for treating neoplasm)

RN 781263-14-3 HCAPLUS

CN Phenol, 3-[2-(hexahydro-1H-azepin-1-yl)-4-(1H-indazol-5-ylamino)-6-pyrimidinyl]- (CA INDEX NAME)

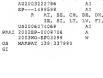


RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 2003:837582 HCAPLUS
DN 139:327990
TI Preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity
IN Previte, Lenard; Van Keulen, Berend Jan; Surtees, John; Talaga, Patrice; Christophe, Bernard
PA UCB, S.A., Belg.
SO PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2003077046	A1	20030918	2003WO-EP02399	20030319 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DM, DK, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU 2003237796	A1	20030923	2003AU-0237796	20030319 <--
EP 1488	A2	20041222	2003EP-0717717	20030319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
US 2006071086	A1	20060406	2003US-0511940	20050106
PRAI 2002EP-0006736	A	20020318		
2003WO-EP02399	W	20030319		

OS MARPAT 139:327990
GI



I

AB Aminopyrimidines I [Y = NHSO2, (un)substituted acetidinyl; R1 = alkyl, cycloalkyl; R2 = cycloalkyl; R3 = H, alkyl, halogen, OH, alkoxy, amino; R1R2 = alkylene; R4 = H, alkyl; R5 = cycloalkyl, aralkyl, heterocyclylalkyl; R6A5 = heterocyclic; combining affinity and inhibitory activity against muscarinic M3 receptors and selectivity as selective phosphodiesterase IV (PDE IV) inhibitors, were prepared. Thus, the amine II was prepared from 4-chloro-N,5-cyclopentyl-6-nitropyrimidin-4-amine by reaction with hexamethylenimine and reduction of the nitro group.

IT 617716-81-3P 617716-84-6P 617716-86-8P
617716-87-9P 617716-88-0P 617717-08-2P
617717-48-2P 617717-50-8P 617717-51-9P
617717-58-6P 617717-63-1P 617717-73-3P
617718-39-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)
(preparation of aminopyrimidines with muscarinic M3 antagonist and PDE IV inhibiting activity)

RN 617716-81-3 HCAPLUS

CN 4-Pyrimidinamine, 2-cyclohexyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- (2E)-2-buten-1-ol (1:1) (CA INDEX NAME)

CM 1

L12 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

CRN 617716-80-2
CMF C18 H28 N4

CM 2

CRN 110-16-7
CMF C4 H6 O4

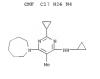
Double bond geometry as shown.

RN 617716-84-6 HCAPLUS

CN 4-Pyrimidinamine, N,5-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl- , (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617716-83-5
CMF C17 H26 N4



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

L11 ANSWER 3 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-17-8
CMF C4 H6 O4

Double bond geometry as shown.

RN 617173-81-8 HCAPLUS
CN 4-Pyridinamine, N-chloro-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617173-80-7
CMF C16 H23 Cl N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-83-0 HCAPLUS
CN 4-Pyridinamine, N,2-dicyclopropyl-5-fluoro-6-(hexahydro-1H-azepin-1-yl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617173-82-9
CMF C16 H23 F N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-84-1 HCAPLUS
CN 4-Pyridinamine, 5-bromo-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617173-85-2
CMF C16 H23 Br N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-86-3 HCAPLUS
CN 4-Pyridinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (2E)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617173-87-4
CMF C17 H25 N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-88-5 HCAPLUS

L21 ANSWER 2 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-84-1 HCAPLUS
CN 4-Pyridinamine, 5-bromo-N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-, (CA INDEX NAME)

RN 617173-85-2 HCAPLUS
CN 4-Pyridinamine, N,2-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

RN 617173-86-3 HCAPLUS
CN N,6-Pyridaltridecalkine, 9H,2-dicyclopropyl-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

RN 617173-88-5 HCAPLUS

L21 ANSWER 2 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
CN 4-Pyridinalkanine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-((1R,2R)-2-methylcyclopropyl)-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617171-11-3
CMF C18 H29 N4

Relative stereochemistry.

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617173-13-2 HCAPLUS
CN 4-Pyridinalkanine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-((1R,2R)-2-methylcyclopropyl)-, rel-(+)- (CA INDEX NAME)

Rotation (+)- Absolute stereochemistry unknown.

RN 617173-89-6 HCAPLUS
CN 4-Pyridinalkanine, 2-cyclopropyl-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

L11 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

● HCl

IT 617718-93-2P
RL: BCT (Reactant); RPH (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 4-aminopiperidines with muscarinic M3 antagonist and PDE IV inhibitory activity)
RN 617718-93-2 HCAPLUS
CN 4-Pyrimidinamine, N,5-dicyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-nitro- (CA INDEX NAME)

IT 617716-99-1P 617717-14-3P 617717-16-5P
617717-17-6P 617717-18-7P 617718-16-2P
617718-57-7P 617718-60-2P 617718-71-5P
RL: BPR (Biological process); BSU (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-aminopiperidines with muscarinic M3 antagonist and PDE IV inhibitory activity)
RN 617716-99-1 HCAPLUS
CN 4-Pyrimidinamine, N-cyclobutyl-2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617716-98-0
CMF C14 H24 N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

Double bond geometry as shown.

RN 617717-14-3 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-2-[(1R,2R)-2-methylcyclopropyl]-, rel-(+)- (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.

RN 617717-16-5 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-5-(cyclopropylmethyl)-6-(hexahydro-1H-azepin-1-yl)-N-methyl-, (2Z)-2-butenedioate (1:1) (CA INDEX NAME)

CM 1

CRN 617717-15-4
CMF C18 H28 N4

CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 617717-17-6 HCAPLUS
CN 4-Pyrimidinamine, 5-chloro-N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 617717-18-7 HCAPLUS
CN 4-Pyrimidinamine, N-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-[(1R,2R)-2-methylcyclopropyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

RN 617718-24-2 HCAPLUS
CN 2H-Azepin-2-one, 3-[2-cyclopropyl-6-(cyclopropylamino)-5-methyl-4-pyrimidinyl]hexahydro- (CA INDEX NAME)

RN 617718-87-7 HCAPLUS
CN 4-Pyrimidinamine, 2-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-5-methyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-86-6
CMF C18 H28 N4

Relative stereochemistry.

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

RN 617718-40-2 HCAPLUS
CN 4-Pyrimidinamine, 5-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-ethyl-N-[(1R,2R)-2-methylcyclopropyl]-, rel-, (2E)-2-butenedioate (2:3) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-56-4
CMF C18 H28 N4

Relative stereochemistry.

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.

RN 617718-73-5 HCAPLUS
CN 4-Pyrimidinamine, 5-cyclopropyl-6-(hexahydro-1H-azepin-1-yl)-2-ethyl-N-[(1R,2R)-2-phenylcyclopropyl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 617718-70-4
CMF C22 H30 N4

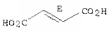
Relative stereochemistry.

L21 ANSWER 2 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CM 2

CRN 110-17-8
CMF C4 H4 O4

Double bond geometry as shown.



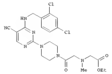
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:796691 HCAPLUS
DN 139:307788
TI Preparation of 5-cyanopyrimidine derivatives as anti-inflammatory agents
IN Machii, Daisuke; Yamaura, Yosuke; Arai, Hitoshi; Yanagawa, Koji; Ohshima, Etsuo; Kawanabe, Ari; Iwase, Miho; Kobayashi, Katsuya; Sato, Takashi; Miki, Ichiro
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003082855	A1	20031009	2003WO-JP04009	20030328 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU2003220968	A1	20031013	2003AU-0220968	20030328 <--
PRAI	2002JP-0090640	A	20020328		
	2003WO-JP04009	W	20030328		

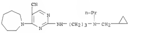
OS MARPAT 139:307788
GI


I


II

AB The title pyrimidine compds. I [wherein R1 and R3 = independently H, OH, halo, (un)substituted alkyl, alkoxy, alkylthio, aryl, aralkyl, or amino; R2 = (un)substituted amino] or ammonium salts or pharmaceutically acceptable salts thereof are prepared as anti-inflammatory agents. For example, the compound II was prepared in a multi-step synthesis. II showed 97% inhibitory activity against thymus and activation-regulated chemokine (TARC) Hut78 cells at 1 μM. Formulations containing I as an active ingredient were also described.
IT 611202-14-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of cyanopyrimidine derivs. as anti-inflammatory agents)
RN 611202-14-3 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 2-[[3-[(cyclopropylmethyl)propylamino]propyl]amino]-4-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

L21 ANSWER 3 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)



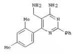
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:656755 HCAPLUS
DN 139:197497
TI Preparation of novel pyridines and pyrimidines as DPP IV inhibitors
IN Boehringer, Markus; Loeffler, Bernd Michael; Peters, Jens-Uwe; Steger, Matthias; Weiss, Peter
PA F. Hoffmann-La Roche A.-G., Switz.
SO PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003068757	A1	20030821	2003WO-EP01107	20030205 <--
	WO2003068757	A9	20041007		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA---2474578	A1	20030821	2003CA-2474578	20030205 <--
	AU2003206833	A1	20030904	2003AU-0206833	20030205 <--
	EP---1476435	A1	20041117	2003EP-0704536	20030205
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
	BR2003007665	A	20050104	2003BR-0007665	20030205
	CN---1630644	A	20050622	2003CN-0803774	20030205
	JP2005526035	T	20050902	2003JP-0567888	20030205
	RU---2293731	C2	20070220	2004RU-0127576	20030205
	US2003216382	A1	20031120	2003US-0361268	20030210 <--
	US---6867205	B2	20050315		
	MX2004PA07744	A	20041015	2004MX-PA07744	20040810
	US2005143405	A1	20050630	2005US-0037989	20050118
	US---7022718	B2	20060404		
PRAI	2002EP-0003114	A	20020213		
	2003WO-EP01107	W	20030205		
	2003US-0361268	A3	20030210		

OS MARPAT 139:197497
GI


I


II

AB The title compds. [I; X = N, CR5; R1, R2 = H, alkyl; R3 = (un)substituted heterocyclyl or aryl; R4 = alkyl, alkoxy, alkylthio, etc.; R5 = H, alkyl], useful for the treatment and/or prophylaxis of diseases which are associated with DPP IV, such as diabetes, particularly non-insulin dependent diabetes mellitus, and impaired glucose tolerance, were prepared and formulated. Thus, reacting benzamidine with 2-(2,4-dimethylbenzylidene)malononitrile in the presence of K_2CO_3 in MeOH followed by treating the reaction residue with $KMnO_4$ in Me_2CO, and reduction of the resulting nitrile with $LiAlH_4$ in THF afforded 7% II which showed IC_{50} of 0.172 μM against DPP IV.
IT 582306-20-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel pyridine and pyrimidine derivs. as DPP IV inhibitors)

L21 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 582306-10-5 HCAPLUS
CN 5-Pyrrolidinecarboxamide, 4-amino-N-(2,6-dichlorophenyl)-2-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

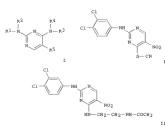
L21 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
R4 = (un)substituted alkyl; R5 = halo; and their pharmaceutically acceptable salts were jerqd. For example, condensation of 3-chloro-2,6-dinitrotoluene (I) with 4-methylpiperidine and 3-chloro-6-(4-methylpiperidin-1-yl)-2-nitrotoluene in one step, and acetylamidoethylamine provided trisubstituted pyrimidine II in 88% yield. In ICK1/Cyclin1 kinase inhibition studies, 99+examples of compds. I exhibited IC50 values more than 100 nM. Compds. I are claimed useful for the treatment of cancer, cardiovascular disease, and inflammation.
IT 314633-45-9P, 2-(1,4-Dichlorophenylamino)-4-(4-oxo-3-propylamino-1-yl)-5-trifluoromethylpyrimidine 314638-46-0P, 4-[2-(3,4-Dichlorophenylamino)-5-trifluoromethylpyrimidin-4-yl]amean-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)
; USES (Uses)
(drug candidate; preparation of trisubstituted pyrimidines as cyclin dependent kinase inhibitors)
RN 314633-45-9 HCAPLUS
CN 5H-Azepin-4-one, 1-[2,4-dichlorophenyl)amino]-5-(trifluoromethyl)-6-pyrimidinyl]hexahydro-3-phenyl- (CA INDEX NAME)

RN 314638-46-0 HCAPLUS
CN 5H-Azepin-4-one, 3-[2-(3,4-dichlorophenyl)amino]-5-(trifluoromethyl)-6-pyrimidinyl]hexahydro- (CA INDEX NAME)

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:319721 HCAPLUS
DN 138:302392
TI Preparation of 2,4,5-trisubstituted pyrimidines as cyclin dependent kinase inhibitors
IN Boehringer, Georg; Emmenlauer, Frank; Wittenberg, Roland; Dudzik, Alexander; Pedinopanic, Anthony A.; Kroth, Heeml, Ashkenpy, Gisely; Steegmaier, Martin; Lenter, Martin, Ackroyd, Andrew; Steurer, Steffen; Sparwik, Walter
PA Boehringer Ingelheim Pharma K.-G., Germany; Boehringer Ingelheim Pharmaceuticals, Inc.; Boehringer Ingelheim International G.m.b.H
SO PCT Int. Appl. , 176 pp
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2003032997	A1	20030424	2002WO-EP11453	20021014 <--
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	CA---2462989	A1	20030424	2002CA-2462989	20021014 <--
	AU2002340496	A1	20030428	2002AU-2340496	20021014 <--
	EP---1438053	A1	20040721	2002EP-0774716	20021014
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE, SK, TR				
	JP2005507924	T2	20050324	2003JP-0539886	20021014
	NZ533715	A	20050729	2003NZ-0533715	20021014
	US---7172029	B2	20070206		
	US---2005065133	A1	20050324	2005US-0133340	20050120
PRAI	DE2001-10151149	A	20011017		
	2003WO-EP11453	W	20021014		
	2002US-0271743	A2	20021016		
OS	MARPAT 138:302392				
GI					



AB Title compds. I [R1 = H, alkyl; R2 = (un)substituted alkyl, R3 = H, alkyl;

L21 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 2003:449648 HCAPLUS
DN 137:133184
TI Preparation of pyrimidinylaminothiocolos as tyrosine kinase inhibitors
IN Hilsman, Mark T.; Hartman, George D.; Hoffman, Zarek W. , Jr.; Luzzio, William C., Jr.; Manley, Peter J.; Rodman, Leonard; Hinkle, John T.; Smith, Anthony M.; Tucker, Thomas J.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 240 pp.
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO2002046452	A2	20020613	2001WO-US45573	20011130 <--
	WO2002046452	A3	20020815		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	US2002137705	A1	20020926	2001US-0990779	20011121 <--
	CA---2419728	A1	20020613	2001CA-2419728	20011130 <--
	AU2002025996	A5	20020618	2002AU-0025996	20011130 <--
	EP---1346040	A2	20030924	2001EP-0997843	20011130 <--
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP2004534082	T	20041111	2003JP-0547438	20011130
	US2004082592	A1	20040401	2003US-0417987	20030602 <--
	US2005119269	B2	20061003		
PRAI	2000US-0251699P	P	20001206		
	2001US-0990779	A1	20011121		
	2001WO-US45573	W	20011130		
OS	MARPAT 137:33318				
GI					

AB Title compds. (I, A, B = N, NO, Y = O, S, NR; R1, R2 = H, perfluoroalkoxy, OH, cyano, halo, (substituted) alkylcarbonyloxyl, (substituted) alkylcarbonyl, (substituted) alkyl, (substituted) aminosulfonyl, (substituted) alkylsulfonyl, (substituted) alkylaminosulfonyl, (substituted) alkoxycarbonyl, (substituted) alkyl, alkenyl, alkynyl, heteroaryl, aminocarbonyl, Re = alkyl, aryl, heteroalkyl;), were prepared for treating angiogenesis, cancer, tumor growth, atherosclerosis, age related macular degeneration, diabetic retinopathy, and hemangiomas. E.g., a multistep synthesis starting with 4-amino-2-chloro-5-pyrimidinecarboxylic acid ethyl ester and 2-amino-4-methylthiazole was reflexed overnight to give 5-methylthiazol-2-yl pyrimidin-4-yl amine. I inhibited vascular endothelial growth factor-stimulated mitogenesis of human vascular endothelial cells with IC50 = 0.91-0.8 nM.
IT 436851-15-9P
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation)
; USES (Uses)
(preparation of pyrimidinylaminothiocolos as tyrosine kinase inhibitors)
RN 436851-15-9 HCAPLUS
CN 5-Thiazolecarbonitrile, 2-[[6-(4-aminobenzoyl)-5H-azepin-1-yl]-4-pyrimidinyl]amino]- (CA INDEX NAME)

L21 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

OTHER ON-MEDIA TAUTOMERIC DOUBLE BONDS NOT DISPLAYED IN THE STRUCTURE

IT 138511-77-7P
RL: PCT (Reactant); SPN (Synthetic preparation); UNEP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinylaminothiazoles as tyrosine kinase inhibitors)

RN 138511-77-7 HCAPLUS

CN Acetamide, N-(5-[4-amino-1-pyrimidinyl]hexahydro-1H-azepin-4-yl)-2,2,2-trifluoro- (CA INDEX NAME)

L21 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 2002:391315 HCAPLUS

DN 136:396130

TI Preparation of pyrimidinylisoform-substituted pyrrolopyridines as inhibitors of cGMP degradation

IN Strach, Johannes-Peter; Porter, Adrian; Weigand, Stefan; Eckel, Elke; Schindler, Udo; Schudt, Christian; Wunder, Frank; Lang, Dieter; Dembowsky, Klaus; Zerwes, Hans-Georg; Alexander, Penelope, Elizabeth

PA Bayer AG, Germany

SO Ger. Offen., 88 pp

CODEN: GWXXBX

DT Patent

LA German

FAN CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI DE- 10123935	A1	20021023	2001DE-10123935	20010514 <--
CA- 2421599	A1	20021030	1891CA-2421599	20011108 <--
WO 2002	A1	20021030	2001WO-EP11965	20011105 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002211917	A1	20021030	2002AU-2002211917	20011105 <--
EP 1339736	A1	20030903	2001EP-997247	20011105 <--
EP 1339736	B1	20041103		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004502085	T2	20040122	2002JP-584633	20011109
ES 2231581	T3	20050516	2001ES-997247	20011105
US 6982283	B1	20060103	2001US-842734	20011109
PRAI DE 2001-10123935	A	20010514		
EP 2001-997247	A	20011031		
2001WO-EP11965	W	20011105		

OS MARPAT 136:396130

GI

AB Title compds. [I; R1 = NH2, NHCO(C1-6 alkyl); R2 = R3NCOR1, R3NCOR4 = substituted heterocyclyl; R3 = H, (substituted) alkyl; R4 = (substituted) heterocyclyl] were prepared. E.g., an 8/3 mixture of 3-(diethylamino)-2-(3-cro-4-morpholinyl)-2-propenenitrile (preparation given) was stirred with 3-(2-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridine-5-carboxamidine (preparation given) in xylene at 110° overnight to give 5-[4-amino-6-[(3-fluorobenzyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-5-pyrimidinyl]-7-morpholinone. Several I showed a vessel relaxation effect with IC50 < 0.25-1.99 μM.

L21 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)

IT 138418-11-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); RCT (Reactant); PREP (Preparation)
(preparation of pyrrolidinylacetam-substituted pyrazolopyridines as inhibitors of cGMP degradation)

RN 138418-11-8 HCAPLUS

CN 3H-Pyrazolo[3,4-d]-1,2,3-triazin-4-[1-[1-(2-fluorophenylmethyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-4-hydroxy-2-pyrrolidinyl]hexahydro- (CA INDEX NAME)

L21 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 1998:141414 HCAPLUS

DN 129:181111

TI Novel pyrimidine antiallergic agents. Part 5: synthesis and pharmacology of pyrimidine amide derivatives

AU Nan, Masakazu; Taguchi, Hiroaki; Katsushima, Takeo; Aoki, Shoichi; Watanabe, Akihiko

CS Pharmaceuticals Research Center, ISHIHARA Co., Ltd., Shiga, 529-0297, Japan

SO Chemical & Pharmaceutical Bulletin (1998), 46(3), 1063-1067

CODEN: CPBTAL; ISSN: 0009-2363

PB Elsevier Science Ltd.

DT Journal

LA English

AB A pyrimidine amide derivs. were synthesized. Novel pyrimidine bis-glycolic amide derivs. showed moderate inhibition in the rat passive cutaneous anaphylaxis (PCA) assay by oral administration. Among these compds., 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine exhibited significant inhibition. However, 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine derivs. substituted with a methyl group or a hydroxyl group at the long fragments of the guinea-pig at less than 10-4 M. Series of 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine have also sizable or moderate activity in the rat PCA assay. An analog which has no oxygen atom at the α-position of the amide carbonyl group and a compound substituted with a methoxy group at the β-position of the amide in the PCA assay it was supposed that both the amide carbonyl group and the oxygen atom at α-position of the amide carbonyl group play an important role in inhibiting the rat PCA reaction. These pyrimidine bis-glycolic amide derivs. have a novel structure and unique activity which suggests they may be clin. very useful in the treatment of allergic diseases.

IT 138418-11-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of pyrimidyl amides as allergy inhibitors)

RN 138418-11-8 HCAPLUS

CN 3H-Pyrazolo[3,4-d]-1,2,3-triazin-4-[1-[1-(2-fluorophenylmethyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-4-hydroxy-2-pyrrolidinyl]hexahydro- (CA INDEX NAME)

L21 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN

AN 1997:542424 HCAPLUS

DN 127:241111

TI Novel antiallergic agents. Part 3: synthesis and pharmacology of pyrimidine amide derivatives

AU Nan, Masakazu; Taguchi, Hiroaki; Katsushima, Takeo; Aoki, Shoichi; Watanabe, Akihiko

CS Pharmaceuticals Research Center, ISHIHARA Co., Ltd., Shiga, 529-0297, Japan

SO Chemical & Pharmaceutical Bulletin (1997), 45(7), 1063-1067

CODEN: CPBTAL; ISSN: 0009-2363

PB Elsevier Science Ltd.

DT Journal

LA English

AB A pyrimidine amide derivs. were synthesized. Novel pyrimidine bis-glycolic amide derivs. showed moderate inhibition in the rat passive cutaneous anaphylaxis (PCA) assay by oral administration. Among these compds., 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine exhibited significant inhibition. However, 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine derivs. substituted with a methyl group or a hydroxyl group at the long fragments of the guinea-pig at less than 10-4 M. Series of 2,4-bis(methoxyacetylamino)-4-piperidinopyrimidine have also sizable or moderate activity in the rat PCA assay. An analog which has no oxygen atom at the α-position of the amide carbonyl group and a compound substituted with a methoxy group at the β-position of the amide in the PCA assay it was supposed that both the amide carbonyl group and the oxygen atom at α-position of the amide carbonyl group play an important role in inhibiting the rat PCA reaction. These pyrimidine bis-glycolic amide derivs. have a novel structure and unique activity which suggests they may be clin. very useful in the treatment of allergic diseases.

IT 138418-11-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of pyrimidyl amides as allergy inhibitors)

RN 138418-11-8 HCAPLUS

CN 3H-Pyrazolo[3,4-d]-1,2,3-triazin-4-[1-[1-(2-fluorophenylmethyl)-1H-pyrazolo[3,4-b]pyridin-3-yl]-4-hydroxy-2-pyrrolidinyl]hexahydro- (CA INDEX NAME)

IT 113259-23-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RACT (Reactant or reagent)

(preparation of pyrimidyl amides as allergy inhibitors)

RN 113259-23-5 HCAPLUS

CN 1,4-Pyrimidinediamine, 6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

RE CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 9 OF 16 BCAPLUS COPYRIGHT 2009 ACS on STN
AN 1997:736641 BCAPLUS
DN 128:13519
TI Preparation of pyrimidinylpiperazines as lipid peroxidation inhibitors
IN Tully, Leroy; Schoenig, Esther; Szilagyi, Katalin; Vuks, Stanislaw; Andrews, Forrest; Sates, Steve; Hodnik, Dexter; Anderson, Tibor; Fehrs, Kevin; Hoffman, Mark; Fehrs, Patrick; Petrelli Schweiger, Laszlo; Szabo, Milko; Stein, Krzysztof; Nowacki, Edit
SO Gyogyszerkutato Intezet, Hung.; Tully, Marie; Tully, Andrea; et al.
SO PCT Int. Appl., 312 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1
PATENT NO. KIND DATE APPLICATION NO. DATE
PI WO--9710685 A1 19970327 1996WO-HU00028 19960916 <--
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, UZ, VN
RW: AT, BE, CH, DE, DK, EA, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SZ, UG
AU--9670455 A 19970407 1996AU-A70455 19960916 <--
AU--9911099 A2 20000330 1999AU-A00088 19990816 <--
PRAI 1995HU-A00252 A 19950919
1996WO-HU00028 A 19960916
OS MARPAT 126:313570
GI

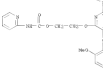
AB Title compds. [I; R = AR(CH2)rC(O)n(CH2)pR1; A = (un)substituted alkylene; R1 = (un)substituted acyl; R2,R3 = NR2 or N-attached heterocyclyl; R = H, OAc, NH2-L (un)substituted amino; r = CH2 or CH(OH); p,q,r = 0 or 1] were prepared. Thus, 1-[1-hydroxy-3-(2-naphthylthio)propyl]piperazine [preparation given] was N-acylated by 2,6-dianilino-4,6-dichloropyrimidine to give I (R = 5,6CH2CH2(NH:CH)2, R1 = 2-naphthyl, R2 = R3 = NH2, n = CH2). Data for 21 I compds. activity of I were given.
IT 186500-77-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinylpiperazines as lipid peroxide. inhibitors)
RN 186500-77-2 BCAPLUS
CN Piperazine, 1-(6-amino-2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl)-4-[(3-hydroxy-2-naphthalenyl)-carbonyl]- (9CI) (CA INDEX NAME)

L21 ANSWER 10 OF 16 BCAPLUS COPYRIGHT 2009 ACS on STN
AN 1997:384169 BCAPLUS
DN 127:177444
TI Synthesis and properties of 2,4-disubstituted 6-fluoropyrimidines
AU Popova, L. M.; Nikonorova, E. P.
CS St. Petersburg Gos. Tekhnol. Inst., St. Petersburg, 198013, Russia
SO Khimiya Geterotsiklicheskikh Soedinenii (1996), 2(10), 1424-1428
CODEN: KGSSAQ; ISSN: 0514-7492
PB Nauka
DT Journal
LA Russian
OS CASREACT 126:277444
AB Reaction of 2,4,6-trifluoropyrimidine, 2-amino-4,6-difluoropyrimidine, and 4-amino-2,6-difluoropyrimidine with amines gave fluoropyrimidines containing two like or unlike amino groups.
IT 189987-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 189987-82-8 BCAPLUS
CN 2-Pyrimidinamine, 4-fluoro-6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

L21 ANSWER 11 OF 16 BCAPLUS COPYRIGHT 2009 ACS on STN
AN 1995:782258 BCAPLUS
DN 123:189847
TI Preparation of sulfonylaminopyrimidines as endothelin antagonists
IN Bres, Volker; Burri, Kaspar; Cotesi, Hans-Marie, Clozel, Martine, Wirth, Georges; Loeffler, Bernd-Michael; Mueller, Marcel, Weidhart, Werner, Ramuz, Henri
PA F. Hoffmann-La Roche AG, Switz.
SO Eur. Pat. Appl., 44 pp.
CODEN: EPXXDW
DT Patent
LA German
FAN.CNT 2
PATENT NO. KIND DATE APPLICATION NO. DATE
PI EP--622059 A1 19941101 1994EP-0100257 19940106 <--
EP--622059 B1 19990113
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
DE--59407538 G 19990225 1994DE-0507538 19940106 <--
CA--2125738 A1 19941029 1994CA-2125738 19940613 <--
CA--2125738 C 20000118
AT------59669 T 19990115 1994AT-0100257 19940106 <--
ES--2127053 T3 19990501 1994ES-0100257 19940106 <--
JP--07010872 A 19950113 1994JP-0126599 19940608 <--
IL----116085 A 19990831 1994IL-0116085 19940613 <--
AU--9465568 A 19950105 1994AU-0065568 19940614 <--
AU--676367 B2 19970306
HU----67634 A2 19950428 1994HU-0001927 19940614 <--
HU--216999 B 19991129 1994HU-0001927 19940614 <--
FI----163744 B1 19940422
NO--9402428 A 19941228 1994NO-0002428 19940627 <--
NO--304432 B1 19981005
BR--9402588 A 19950228 1994BR-0002588 19940627 <--
CN--1106207 A 19950802 1994CN-1106074 19940627 <--
CN--1058039 B 20000223
US--5514674 A 19960507 1996US-0601870 19960207 <--
US----11178 B 19980430 1998US-0800131 19970217 <--
US--5541184 A 19960730 1996US-0666072 19960627 <--
FI----119731 B1 19981204 1998FI-0002680 19981207 <--
FI----117033 B1 19990930 1999FI-0923896 19991027 <--
FI----117034 B1 19990930 1999FI-0923897 19991027 <--
CZ----291164 B6 20021113 1996CZ-0001833 19961227 <--
JP--07317972 A 19981110 1998JP-0194203 19980628 <--
JP----2966200 B2 19991025
RO----113439 B1 19980330 1995RO-0001112 19951020 <--
RU--2107690 C1 19980327 1995RU-0109779 19950614 <--
PRAI 1993EP-0201514 A 19930218
1993IL-0106490 A2 19930630
1994GB-0000178 A 19940105
OS MARPAT 123:36947
GI

AB Title compds. [(i. R1-R3 = H, alkyl, alkoxy, alkylthio, alkenyl, halo, CF3, hydroxyalkoxy, haloalkoxy, alkoxyalkyl, hydroxyalkyl, OSO2R, amino, wh. = NIR1, R2R3, R4C(= O)NR5(alkyl), methylenedioxy, ethylenedioxy, isopropylidenedioxy, R4 = H, alkyl, cycloalkyl, CF3, alkoxy, alkynyloxy, alkylthio, alkylthioalkyl, hydroxyalkyl, dihydroxyalkoxy, alkylsulfonyl, alkylaminoalkyl, aryl, arylthio, aryloxy, heteroaryloxy, heterocyclylalkyl, heterocyclyloxy, R5 = H, alkyl, alkenyl, alkynyl, cycloalkyl, alkylaminoalkyl, R4, R5 = H, alkyl, alkoxy, alkylthio; X = O, S, CH2, > C(CH3)2, HNCH2CH2O, O2CCH2S, HNCH2O2S; R16 = alkyl, cycloalkyl,

L21 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
nyticoxyalkyl, corticoxyalkyl, alkoxycarbonylalkyl, alkoxyoxyalkyl, arylcarbonylalkyl, heteroaryloxyl, heteroarylalkyl, etc.; R11 = H, R12, m = 1-3, n = 0,1), were prepd. Thus, 2-pyridinecarboxyl azide was heated in PhCNO, 4-methyl-N-(4-(2-hydroxyethoxy)-6-(2-methoxyphenoxy)-2,2'-bipyrimidin-4-yl)benzenesulfonamide was added to give pyrimdine-2-carbamate, which was treated with 2-methoxyphenol and 4-(2-methoxyphenoxy)-2,2'-bipyrimidin-6-yl-ethyl ester. The latter at 30 mg/kg orally in rats gave a 30% redn. in ex- actarial blood pressure
IT 167014-84-4P
RL: BAC (Biological activity or effector, except adverse); MAM (Biological activity, miscellaneous); PAC (Pharmacological activity); PREP (Preparation); USES (Uses)
(prepn.-action of sulfonylaminopyrimidines as endothelin antagonists)
RN 167014-84-4 HCAPLUS
CN Benzenesulfonamide, 4-methyl-N-[4-[6-[(1,3-benzodioxol-5-ylmethyl)amino]-2-(hexahydro-1H-azepin-1-yl)-5-(2-methoxyphenoxy)-4-pyrimidinyl]-2-(2-methoxyphenoxy)-4-pyrimidinyl]methyl ester (9CI) (CA INDEX NAME)



L21 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 1991:454199 HCAPLUS
DN 115:54199
TI Preparation of N-sulfonylpyrimidine ester salts and pyrimidine N-oxides as heat loss retardants
IN Dufvelt, Didier; Entremer, Francoise; Goetsch, Quintino; Hoogmans, Michel
PA Ucb
SO Ger. Offen., 49 pp.
CODEN GWXXBX
DT Patent
LA French
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI CA----2024596	A1	19910301	1990CA-2024596	19900829 <--
CA----2024596	C	20030121		
EP----0415907	A1	19910306	1990EP-0810352	19900829 <--
FR----2651122	A1	19910228		
EP----470707	A1	19910603	1990ED-8402361	19900814 <--
EP----470707	B1	19931215		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT----98977	E	19940115	1990AT-0402361	19900814 <--
JP----03114972	A	19910522	1990JP-0232631	19900824 <--
JP----3052209	B2	20000619		
CA----2085896	C	20070101	1990CA-2085896	19900828 <--
ES----2061002	A	19971101	1991ES-0661849	19910405 <--
ES----2061002	B1	19980216	1994ES-3765113	19941216 <--
PRAI 1989FR-0011352	A	19890901		
1990EP-0402361	A	19900814		
1990ES-0765178	A1	19900817		
1990CA-2024596	A3	19900828		
1994ES-3765113	A3	19940407		
OS MARPAT 115:154199				
GI				

AB Title compds. [(; R = H, alkyl; R11 = H; R811 = (CH2)3-5; R12 = H, alkenyl, alkoxycarbonyl, substituted CONR2; R' = H, NHLR2, alkoxy, alkylthio, PhO, etc.; R1, R2 = H, cycloalkyl, alkenyl, (un)substituted Ph, etc.; NR1R2 = heterocyclyl; Y = O, OSO2- (N has pos. charge)] were prepared as hair loss retardants (no data). Thus, 2-amino-4-methyl-6-(hexahydro-1H-azepin-1-yl)pyrimidine (I) and 2-chloro-4-methyl-6-(hexahydro-1H-azepin-1-yl)-1-oxidopyrimidine (II) complex to give title compound II.
IT 137716-17-7P 137716-16-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as hair loss retardant and growth stimulant)
RN 137716-17-7 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl-, 1-oxide (CA INDEX NAME)

L21 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 1991:159568 HCAPLUS
DN 114:159568
TI Preparation of pyrimidinium derivatives as cardiovascular agents
IN Hargreaves, Rodney Brian; McConnalin, Bernard Joseph, Mills, Stuart Bennett
PA Imperial Chemical Industries PLC, UK
SO Eur. Pat. Appl., 31 pp.
CODEN EPXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP----434341	A1	19910626	1990EP-0313770	19901217 <--
EP----434341	B1	19950517		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU----56097	A2	19910728	1990HU-0008116	19901207 <--
HU----208111	B	19930928		
CA----2050951	A	19910630	1991CA-2050951	19910207 <--
AU----9067914	A	19910627	1990AU-0067914	19901210 <--
AU----641940	B2	19931007		
NO----3105378	A	19910626	1990NO-0005378	19901213 <--
NO----174263	B	19940124	1990NO-0005378	19901213 <--
ZA----9010367	A	19910912	1990ZA-0010367	19901218 <--
CA----2022743	A1	19910623	1990CA-2022743	19901219 <--
FI----9106298	A	19910623	1991FI-0906298	19901220 <--
JP----03291277	A	19911220	1991JP-0404324	19901221 <--
PRAI 1989GB-0029023	A	19891222		
OS MARPAT 115:159568				
GI				

AB Title compds. I (R1 = C1-10 alkyl, C3-8 cycloalkyl; (substituted) Ph, PhCH2, 5-6 membered heterocyclyl; R2 = C1-10 alkyl, C3-8 cycloalkyl, C2-4 alkenyl; R4 = C1-4 alkyl, NIR, C1-4 alkylamino; R3, R5 = H, C1-4 alkyl, (substituted) Ph, NvCH2, A, B = CH2CH2, (CH2)3; E = bond, O, S, CO, CH2, etc.; Y = anion), were prepared 3-methyl-4-(methylamino)-6-(5-phenylpiperidinoyl)pyrimidine (preparation given) and HeI in dioxane were refluxed 1 h to give 1,3-dimethyl-4-(methylamino)-6-(5-phenylpiperidinoyl)-2-pyrimidinium iodide (structure in heating coil of nonstreamsly heating isolated pig right atrium). A capsule and tablet formulation comprising 1 ere given.
IT 136346-41-7P
RL: SPN (Synthetic preparation); PREP (Preparation), PACT (Pharmacological activity); RACT (Reactant or reagent)
(preparation and quaternization of, with Me iodide)
RN 136346-41-7 HCAPLUS
CN 4-Pyrimidinamine, 6-(hexahydro-1H-azepin-1-yl)-N,2-dimethyl- (CA INDEX NAME)

IT 136346-34-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU

L21 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
RN 137716-16-1 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl-1-(sulfooxy)- (CA INDEX NAME)

L11 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
(Therapeutic use); RCTV (Biological activity); PREP (Preparation); USES (Uses)
(preps. of, as cardiovascular agent)
RN 134246-31-6 HCAPLUS
CN Methanesulfonic, N-(N-(hexahydro-1H-azepin-1-yl)-1,2,5-dimethyl-4(1H)-pyrimidinylidene)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L11 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2009 ACS on STN (Continued)
5-methyl-amino-3-(4-phenylpiperidin)pyridine. The latter in THF contg. BuLi was treated with PhCOCl in THF and then with pyridine. The mixt. was refluxed 1 h to give 3-(4-benzoyl-4-phenylpiperidin)-5-methylamino in 74% with oxalate salt; serves from 22.3% of normal (controls) to of 1-24 2% at 10-32 mg/kg i.p. daily over 30 d..
IT 131027-57-0P 131030-03-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(preps. of, as cardiovascular nervous system agents)
RN 131027-57-0 HCAPLUS
CN Benzamide, N-(2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl)-N-methyl- (CA INDEX NAME)

RN 131028-42-3 HCAPLUS
CN Benzamide, N-(2-(hexahydro-1H-azepin-1-yl)-4-pyrimidinyl)-N-methyl-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L21 ANSWER 14 OF 26 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 1991:23963 HCAPLUS
DN 114:23963
TI Preparation of 2-aminopyrimidines as nervous system agents
IN Tomio, Ikuo; Ichesue, Mitsuyuki; Eshete, Morizki; Eii-Ohete, Sokumi; Awano, Akira; Horikawa, Kazutoshi; Sasaki, Tadayuki; Miyachi, Shiro
PA Yoshitomi Pharmaceutical Industries, Ltd., Japan; Mitsui Pharmaceuticals, Inc.
SO Ger. Offl. Appl., 154 pp.
CODEN: EOXXDW
DT Patent
LA English
FAN CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP----379096	A2	19900801	1989EP-0133595	19891227 <---
EP----379096	A3	19910529		
EP----379096	B1	19950125		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP--02221375	A	19900904	1989JP-0041729	19890223 <---
JP----3017849	A2	19910128	1989JP-0304941	19891122 <---
JP----3063377	B	19912108		
US--5021418	A2	19910604	1990US-0501485	19900330 <---
US--5100901	A	19920331		
WO---61312	A2	19911228	1991WO-US01657	19910312 <---
WO---205574	B	19940825		
WO---61298	A3	19912128	1991WO-US01670	19910312 <---
WO---205575	B	19940825		
JP--03214568	A	19910213	1989JP-0324753	19891206 <---
JP--2744863	B2	19980428		
EP----412796	A1	19940831	1990EP-0310918	19900727 <---
R: DE, FR, GB, IT				
AT----379096	T	19980415	1989AT-0133595	19891227 <---
AU----6417325	A	19900705	1989AU-0617325	19891228 <---
AU----629595	B2	19921008		
CA--2006744	A1	19900629	1989CA-2006744	19891225 <---
CN---1043203	A	19900711	1989CN-0109731	19891223 <---
CN---1021178	B	19930616		
US--5167676	A	19921201	1989US-0450376	19891229 <---
US--5284435	A	19931102	1991US-0789736	19911104 <---
CN---1050846	A	19910417	1991CN-1011389	19910401 <---
PRAI 1988JP-0333470	A	19881223		
1989JP-0041729	A	19890223		
1989JP-0061703	A	19890313		
1989JP-0324753	A3	19891223		
1989EP-0133595	A3	19891227		
1989US-0450376	A3	19891229		

OS MARPAT 114:23963
GI

AB The title compds. [I; R1 = H, alkyl; X = morpholino, (substituted) piperidino, hexamethyleneimino, (substituted) piperazino, (substituted) tetrahydroisoquinolinyl, etc.; Y = amino, pyridin-4-ylcarbonyl, piperidinyl-N-carbonyl, phenylcarbamoyl, benzoyl, phthalimido, etc., CH2R1; R2 = H, alkyl, alkoxy, alkylthio, dialkylamino; Z = H, halo, alkyl, alkoxycarbonyl], were prepared 2Bzo MeNH2 in MeOH was added to 2,4-dichloropyrimidine in CH2Cl2 at 5° followed by stirring for 1 h at room temperature to give 4-chloro-2-methylaminopyrimidine The latter was heated with 4-phenylpiperidine in BuOH at 120° for 2 h to give

L21 ANSWER 15 OF 26 HCAPLUS COPYRIGHT 2009 ACS on STN
AN 1988:193353 HCAPLUS
DN 109:193353
TI Synthesis of new substituted 5,6-dihydrotetrazolo[1,5-c]quinazolines, tetrazolo[1,5-c]quinazolines, 5,6-dihydropyrazolo[5,4-e]tetrazolo[1,5-c]pyrimidines, and 5,6-dihydrotetrazolo[1,5-c]pyrimidines
AU Hiel, Walter; Abou-Setouh, Saleh
CS Inst. Org. Chem., Univ. Frankfurt, Frankfurt/Main, D-6000/70, Fed Rep Ger
SO Chemiker-Zeitung (1988), 112(4), 133-40
CODEN: CHEIAJ; ISSN: 0009-2894
DT Journal
LA German
OS CASREACT 109:193353
GI

AB 5,6-Dihydrotetrazolo[1,5-c]quinazolines I (R = H, Cl, OCH3, R1 = OCl3, CH2(CH2)m-3-3,4,5, CH4H2CNH-4, CH4CCl-5,6, CH4Cl-4; R2 = H) were prepared by cyclocondensation of tetrazolylanilines II with RICNO. I (R = H, Cl, OCH3; R1 = Me, Ph; R2 = H, Me, CONH2, CH2CONH2) were prepared by cyclocondensation of II with R1COR2. 5,6-Dihydropyrazolo[5,4-e]tetrazolo[1,5-c]pyrimidines III (R = H, Cl, OCH3; R1 = piperidino, morpholino, hexahydro-1H-azepin-1-yl; R3 = H, Me, CH2(CH2)m-4, CH4CCl-2,6, CH4Cl-4, CH4NH2-4, CH4Cl(me)-3,4,5, CH4NH2-5) were prepared by cyclocondensation of 4-substituted-5-pyrazolylpyrimidines IV with R1COR. 5,6-Dihydrotetrazolo[1,5-c]pyrimidines V (R5 = H, Me, NH2; R6 = Me, CH2(CH2)m-3-3,4,5, CH4NH2-4, CH4Cl(me)-3,4,5, CH4Cl-5) were prepared from nitriles VI and NaCNO.
IT 117096-59-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with azide, tetrazole derivative from)
RN 117096-59-0 HCAPLUS
CN 5-Pyrimidinecarbonitrile, 4-amino-2-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

L11 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
IT 111695-15-3P
RL: PCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of, and cyclocondensation of, with aldehydes)
RN 111695-15-3 HCAPLUS
CN 4-Pyrimidinamine, 5-(hexahydro-1H-azepin-1-yl)-4-(3H-tetrazol-5-yl)- (9CI)
(CA INDEX NAME)

L21 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1988:112484 HCAPLUS
DN 108:112484
TI Preparation of heterocyclylpyrimidinediosmates as allergy inhibitors
IN Taguchi, Hiroshi; Katsuhima, Takeo; Ban, Masakazu; Aoki, Shoichi, Japan
PA Yoshitomi Pharm. Ind., Japan
SO Ger. Offen., 21 pp
CODEN: EOXXDW
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI EP---242817	A1	19871104	1987EP-105967	19870416 <---
R: AT, BE, CH, DE, FR, IT				
US---4879284	A	19891024	1987US-0033734	19870403 <---
JP---63264364	A	19881101	1987JP-0093615	19870416 <---
PRAI 1986ZP-0081482	A	19860411		
1986JP-0107840	A	19860512		
OS CASREACT 108:112484, MARPAT 108:112484				
GI				

AB The title compds. [I; R1, R3 = H, alkyl, PhCH2, alkali metal cation, NH4+; R2 = H, halo, alkyl, alkoxy, aryl, NH2, (heterocyclic amino) were prepared as allergy inhibitors. 2,4-Diamino-6-piperidinopyrimidine in pyridine was condensed with Et oxalyl chloride with initial cooling. The mixture was refluxed 1 h with continued cooling, temperature to give 1 (R1 = R3 = H, R2 = piperidino) (II). At 1 mg/kg i.v. in rats, II gave 50 wk inhibition of passive cutaneous anaphylaxis.
IT 113269-35-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by alkyl oxalyl chloride, in preparation of allergy inhibitors)
RN 113269-35-9 HCAPLUS
CN 2,4-Pyrimidinediamine, 6-(hexahydro-1H-azepin-1-yl)- (CA INDEX NAME)

IT 113258-20-6P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as allergy inhibitor)
RN 113258-20-6 HCAPLUS
CN Acetic acid, 2,2'-[[6-(hexahydro-1H-azepin-1-yl)-2,4-pyrimidinediyl]diimino]bis[2-oxo-, dimethyl ester (9CI) (CA INDEX NAME)

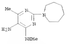
L21 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L21 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1978:443304 HCAPLUS
DN 89:43304
ORP 89:7323a,7326a
TI Study of Lactam. XXIX. Synthesis and some reactions of 3-oxo-3,4-dihydroxy-4-bromobenzhydroxamines
AU Glushkov, R. G.; Smirnova, V. G.; Zaozerova, I. N.; Sterkhin, Z. V.; Ovcharova, I. M.; Vlasova, Z. P.
CS Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR
SO Khimiya Geterotsiklicheskikh Soedinenii (1978), (3), 374-8
CODEN: KGSSAQ; ISSN: 0453-8734
DT Journal
LA Russian
OS CASREACT 89:43304
GI

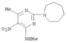
AB Condensation of the title compound I with o-ZOHC6H4OH gave 33-77% II (R = H, Et, PhCH2, meCHCH2CH2, ElCHCH3CH2). Treatment with ElSO4-HF+ gave 87 and 49% III (R = EC, PhCH2). Pyrimidopyrrolizinequinone IV (R = Me, R, R1 = Me; R = Me, R1 = H) were obtained in 4-55% yields by condensation of I with 2-aminopyrrole-3-carboxylic acid derivs. Hydrolysis of I with thiourea gave 76% V and condensation with MeCHCHCOCOH gave 62% VI.
IT 66751-44-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 66751-44-8 HCAPLUS
CN 2,4(1H,3H)-pyrimidinedione, 6-amino-3,5-dimethyl-5-(2,5,6,7-tetrahydro-3-hydroxy-2-oxo-1H-azepin-4-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

L21 ANSWER 18 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1976:17283 HCAPLUS
DN 84:17283
OREF 84:2863a,2866a
TI Purine studies. XVII. Synthesis of 2-substituted 6,9-di- and 6,8,9-trimethylpurines as amplifiers of phleomycin
AU Bhushan, Kul; Brown, Desmond J.; Lister, John H.; Stephanson, Lawrence G.; Yoneda, Fumio
CS John Curtin Sch. Med. Res., Canberra, Australia
SO Australian Journal of Chemistry (1975), 28(11), 2553-9
CODEN: AJCHAS, ISSN: 0004-9425
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB 2-(6,8,9-Trimethylpurin-2-ylthio)acetamide (I, R = SCH2CONH2, R1 = Me) and analogous N-substituted acetamides are prepared by treatment of 6,8,9-trimethylpurine-2-thione with an appropriate 2-chloroacetamide. 6,9-Dimethyl-2-(piperidin-1-yl)purine I(R = piperidino, R1 = H) and some 2-polymethyleneamino homologues are mede by initial amination of 2-chloro-4-methyl-6-methylamino-5-nitropyrimidine followed by reduction of the nitro group and final cyclization with HCO2H. Such purines enhance the lethal effect of phleomycin on Escherichia coli cultures
IT 57880-52-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, purine derivs. from)
RN 57880-52-1 HCAPLUS
CN 4,5-Pyrimidinediamine, 2-(hexahydro-1H-azepin-1-yl)-N4,6-dimethyl- (CA INDEX NAME)



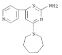
IT 57880-51-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 57880-51-0 HCAPLUS
CN 4-Pyrimidinamine, 2-(hexahydro-1H-azepin-1-yl)-N,6-dimethyl-5-nitro- (CA INDEX NAME)



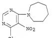
L21 ANSWER 19 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:140173 HCAPLUS
DN 82:140173
OREF 82:22399a,22402a
TI 2,4,6-Trisubstituted pyrimidines
IN Tani, Hideo; Nakamura, Koji; Mori, Shizuhiro; Yokoo, Nobuo; Kyotani, Yoshitoku; Wada, Yasushi
PA Kowa Co., Ltd
SO Jpn. Tokkyo Koho, 12 pp.
CODEN: JAXXAD
DT Patent
LA Japanese
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP--49021148	B	19740530	1970JP-0127609	19701228 <--
PRAI	1970JP-0127609		19701228		

GI For diagram(s), see printed CA Issue.
AB Sixty-three antiinflammatory (no data) pyrimidines (R = 4-pyridyl, Ph, etc., R1 = NH2, NMe2, NEt2, morpholino, NHPr, piperidino, OMe, etc.; R2 = NMe2, OCH2CH2NMe2, NEt2, morpholino, NHCH2CH:CH2, NHCH2CH2OH, etc.) were prepared by reacting I (R1 = SO2Me or Cl) with the appropriate amine or alc. E.g., I (R = NH2, R1 = SO2Me, R2 = 4-pyridyl) (0.016 mole) was refluxed 1 hr with 30 ml MeOH containing 0.03 mole Na to give 80% I (R = NH2, R1 = OMe, R2 = 4-pyridyl).
IT 54993-89-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54993-89-4 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-1-yl)-6-(4-pyridinyl)- (CA INDEX NAME)



L21 ANSWER 20 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1975:4203 HCAPLUS
DN 82:4203
OREF 82:727a,730a
TI Heterocyclic studies. XXXI. New routes to reduced imidazole, pyrimidine, and pyridopyrimidine derivatives
AU Clark, Jim; Curphey, Michael; Southon, Ian W.
CS Ramage Lab., Univ. Salford, Salford, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1974), (14), 1611-14
CODEN: JCPRB4, ISSN: 0300-922X
DT Journal
LA English
GI For diagram(s), see printed CA Issue.
AB Six 4-(substituted amino)-6-chloro-5-nitropyrimidines [I, e.g. R = NEtPh, NH(CH2)2OH] with dilute AcOH gave RC(NH2):C(CN)NO2. I [R = NMe(CH2)2OH] with POCl3 followed by H2O gave the reduced imidazole II (R = Me) via the quaternary salt III. Similarly I [R = N[(CH2)2Cl]2] gave II [R = (CH2)2Cl] and I [R = NPh(CH2)3OH] gave the hexahydropyrimidines IV (R = H and CHO), and 4-chloro-6-[2-(2-hydroxyethyl)piperidino]-2-methyl-5-nitropyrimidine gave the pyridopyrimidine V.
IT 54413-32-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and ring cleavage of)
RN 54413-32-0 HCAPLUS
CN 1H-Azepine, 1-(6-chloro-5-nitro-4-pyrimidinyl)hexahydro- (CA INDEX NAME)



L21 ANSWER 21 OF 26 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1969:115172 HCAPLUS
DN 70:115172
OREF 70:21518h,21519a
TI 1,2-Dihydro-1-hydroxy-2-imino-6-methyl-4-(dialkylamino)pyrimidines and 1,6-dihydro-1-hydroxy-6-imino-2-methyl-4-(dialkylamino)pyrimidines
IN Ursprung, Joseph J.; Anthony, William C.
PA Upjohn Co.
SO Fr., 38 pp.
CODEN: FRXXAK
DT Patent
LA French
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR---1513739	A1	19680216	1967FR-0095687	19670220 <--
PRAI	1966US-0528790	A	19660221		

OS MARPAT 70:115172
GI For diagram(s), see printed CA Issue.
AB 2-Amino-6-methyl-4-(R-substituted)-5-(R1-substituted)-pyrimidines (I) and 6-amino-2-methyl-4-(R-substituted)-5-(R1-substituted)-pyrimidines (II), where R is an aryloxy group, are treated with HOOAc and m-ClC6H4C(O)OOH to give 1,2-dihydro-1-hydroxy-2-imino-4-(R-substituted)-5-(R1-substituted)-pyrimidines (III) and 1,6-dihydro-1-hydroxy-6-imino-4-(R-substituted)-5-(R1-substituted)-pyrimidines (IV). III and IV, where R is an aryloxy group, are treated with amines to give 4-amino compds. Thus, 28.6 g. I (R = Cl, R1 = H) is treated with 94 g. PhOH in the presence of KOH at 95-100° to give 79% 2-amino-6-methyl-4-phenoxypyrimidine (V), m. 192-4°. A solution of 14.2 g. V and 0.14 mole HOOAc in 150 ml. HOAc is heated 20 hrs. at 58° to give 28% 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-phenoxypyrimidine (VI), m. 190-3°. VI (1.0 g.) is added to a solution of 0.96 g. Na and 0.005 g. FeCl3 in 20 ml. piperidine, and the mixture refluxed 2 hrs. to give 41% 1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-piperidinopyrimidine. Similarly prepared are I (R = 2,4-Cl2C6H3O, R1 = H), m. 195-6°; I = (R = 2,4-Cl2C6H3O, R1 = Me), m. 157-8°; the following III (R, R1, and m.p. given): 2,4-Cl2C6H3O, H, 216-18°, piperidino, H, 260-1°; pyrrolidino, H, 271-3°; morpholino, H, 261° (decompose 264-7°), 4-methyl-1-piperazinyl, H, 212-13° (2,4-Cl2C6H3OH salt m. 151-2°); hexamethylenimino, H, 208-10°; Me2N, H, 228-9°; CH2:CHCH2NH, H, 252-5° (decomposition), PhCH2NH, H, 227-9°; 2,4-Cl2C6H3O, Me, 225-6°, piperidino, Me, 172-3°, 2,4-Cl2C6H3O, Br, 212-14°; pyrrolidino, Br, 166-7°; II (R = 2,4-Cl2C6H3O, R1 = H), m. 157-8°, and the following IV (R, R1, and m.p. given): 2,4-Cl2C6H3O, H, 214-16°, piperidino, H, 200-200.5°; 2,4-Cl2C6H3O, Br, -, pyrrolidino, Br, -. III (R1 = Br) and IV (R1 = Br) are treated with amines and thiophenols to give the following III (R, R1, and m.p. given): pyrrolidino, pyrrolidino, 224-6°; pyrrolidino, piperidino, - (monohydrate m. 204-6°), pyrrolidino, p-ClC6H4S, 169-70°, and the following compds.: IV (R = R1 = pyrrolidino), IV (R = pyrrolidino, R1 = p-ClC6H4S). A mixture of 5.4 g. III (R = pyrrolidino, R1 = Br) and 50 ml. pyrrolidine is heated 3 hrs. at 108-10° to give III (R = pyrrolidino, R1 = H) and III (R = R1 = pyrrolidino), m. 186-7°, in a 1:1 weight ratio. Also prepared, according to known methods (halogenation, nitration, NO2 group reduction, acylation), are the following compds. (m.p. given): I (R = 2,4-Cl2C6H3O, R1 = Br), 155-6.5°, III (R = piperidino, R1 = NO2), 196-9°, III (R = piperidino, R1 = NH2), -, II (R = 2,4-Cl2C6H3O, R1 = Br), -, IV (R = piperidino, R1 = NO2), -, IV (R = piperidino, R1 = NH2), -, III (R = piperidino, R1 = H) HCl, -, and 1,2-dihydro-1-hydroxy-2-acetylimino-6-methyl-4-piperidinopyrimidine, -. Uv and ir data are given. (In this abstract, pyrrolidino-1-pyrrolidinyl.)
IT 22370-34-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 22370-34-9 HCAPLUS
CN 1H-Azepine, 1-(1,2-dihydro-1-hydroxy-2-imino-6-methyl-4-pyrimidinyl)hexahydro- (8CI) (CA INDEX NAME)

L21 ANSWER 21 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L21 ANSWER 22 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1968:83167 HCAPLUS
DN 68:83167
ORIG 68:17749-a,17749-h
TI Tetrazolo-allylazamethine rearrangements in pyrimidine series
AU Piotrovskii, L. Ya.; Smirnova, N. N.
CS S. M. Kirov Polytech. Inst., Sverdlovsk
SO Doklady Akademii Nauk SSSR (1968), 180(5), 1134-9
CODEN: DANKAS, ISSN: 0002-3264
DT Journal
LA Russian
SI File diagram(s), see printed CA Issue.
AB Addition of NCBrz NZO to 4,6-dichloropyrimidine in MeOH (exothermic) rapidly gave 4,6-dichloro-5-bromopyrimidine (I), m. 73-4°. I reacted with aqueous amines 2 hrs. gave 4,6-di-R-5-bromopyrimidines (substituent shown): morpholino, m. 144-7°; N-homopiperidinyl, m. 134-7°; N-pyrrolidinyl, m. 155-8°; piperidino, m. 122-3°. Three treated with 2N HCl, followed by aqueous NaNO3 at 0° gave 4,6-di-R-5-nitropyrimidines (substituent shown): morpholino, m. 93-5°; N-homopiperidinyl, m. 81°. The remaining mono meta converted by this reaction into tetrazolo[1,5-c]-substituted-pyrimidines (II): N-pyrrolidinyl, m. 87°; piperidino, m. 77-8°. Ir spectra are shown. Thus, the presence of only electron-donor substituents in the pyrimidine molecule favors the production of the tetrazole structure, existing only in the azide form in the above procedure; in solution these were equilibrated with the azides (III), as shown spectroscopically
IT 5767-10-8
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 5767-10-8 HCAPLUS
CN 1H-Azepin, 1-(4-azido-4-pyrimidinyl)hexahydro- (CA INDEX NAME)

IT 5767-37-3D, Hexamethylenimine, 1-(4-hydrazino-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 5767-37-3 HCAPLUS
CN 1H-Azepin-4-amine, N-(hexahydro-1H-azepin-1-yl)-, hydrazone (9CI) (CA INDEX NAME)

L21 ANSWER 23 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:40241 HCAPLUS
DN 53:40241
ORIG 53:7709-i
TI Pyrimidines
PA Societe des usines chimiques de Rhone-Poulenc
SO Add. to Fr. 1,058,836 (C.A. 53, 14386a)
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR----1063796		19560120	FR	----
CH----360019			CH	
DE----1039111			DE	
GB----1015786			GB	
PRAI US		19541207		

AB 4-Methyluracil deriva. were prepared and used in herbicidal compns. Thus, a mixture of 3-(hexahydro-1-azepinyl)urea 128, Et acetoacetate 104, and 2 drops concd. HCl was heated 1 hr. at 100° and cooled to 0°. A 26% NaOMe-MeOH solution (192 parts) was added to the cooled solution, and heating continued 3 hrs. The mixture was cooled, shaken with 1N (1000 parts), separated, and the organic layer shaken with H2O. The combined aqueous layers were washed with CHCl3. Acidification of the aqueous layers precipitated 3-(hexahydro-1-azepinyl)-6-methyluracil, m. 260°. A mixture of 3 parts of a solution of 11.3 parts I and 18 parts glycerol-NaAc in 100 parts MeAc at 30°. The solution was shaken for a further 30 min. and poured into H2O (160 parts) to precipitate 5-chloro-3-(hexahydro-1-azepinyl)-6-methyluracil. Also prepared from I were the following 3-(hexahydro-1-azepinyl)-6-methyluracils (substituent shown): 5-bromo, m. 260°; 5-methoxy, m. 245°; 5-methoxymethyl, 1-methyl. Also prepared was 3-(hexahydro-1-azepinyl)-6-methyl-4-thiouracil. Other compds. claimed were: 5-bromo-6-methyl-3-(1-piperidinouracil; 5-chloro-6-methyl-3-(1-piperidino)uracil; 5-bromo-6-methyl-3-(pyrrolidinyl)uracil; 5-chloro-6-methyl-3-(1-pyrrolidinyl)uracil; 5-bromo-6-methyl-3-(hexahydro-1-azepinyl)uracil; 6-methyl-3-(4-morpholino)uracil.

IT 14788-51-0
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 14788-51-0 HCAPLUS
CN Uracil, 3-(hexahydro-1H-azepin-1-yl)-4-methyl-5-nitro- (6CI) (CA INDEX NAME)

L21 ANSWER 24 OF 36 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1959:40241 HCAPLUS
DN 53:40241
ORIG 53:7709-i
TI Pyrimidines
PA Societe des usines chimiques de Rhone-Poulenc
SO Add. to Fr. 1,058,836 (C.A. 53, 14386a)
DT Patent
LA Unavailable
FAN.CNT 1

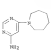
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI FR----43159		19550825	FR	19518723 ---

AB 4-Aminopyrimidines corresponding to substituted phenyl and 6-methyl-2-amino groups are prepared as in the main patent. Thus, 8 g. 2,4-diamino-5-(3,4-chlorophenyl)-4-chloropyrimidine autoclaved 7 hrs. at 200-10° with 34 cc. NaOMe in 58 cc. EtOH gave 2,4-diamino-5-(3,4-chlorophenyl)-6-dimethoxypyrimidine, m. 134-7° (aqueous EtOH), also obtained by autoclaving 2,4-diamino-5-(3,4-chlorophenyl)-6-chloropyrimidine 6 hrs. at 200-10° with EtOH and NaOH. Similarly were obtained derivs. bearing at position 6 the following groups: MeCH2, m. 212-13°; EtCH2, m. 208°; MeCH, m. 125-26°; EtCH, m. 142-3°; piperidino, m. 136°; hexamethylenimino, m. 153°; N-methylanilino, m. 160°; and PhCH2O. 2,4-Diamino-5-(3,4-dichlorophenyl)-6-methylpyrimidine m. 140-50°. Similarly PhCH2O and the 5-(3,4-dichlorophenyl compound give 2,4-diamino-5-(3,4-dichlorophenyl)-6-dibutylaminopyrimidine, m. 104°. 2,4-Diamino-5-phenyl-6-chloropyrimidine (I) (27 g.) autoclaved 8 hrs. at 200° with 74 cc. EtOH and 200 g. NH3 gives, on cooling, 2,4,6-triamino-5-phenylpyrimidine (II), m. 240° (EtOH); II crystallizes with 1H2O in colorless needles, m. 90-5°, following dehydration; treated with NBrAN, II gives 2,4,6-triamino-5-phenylpyrimidine (III), m. 241° (EtOH); II treated with HNO2 in concentrated HClAn at -15° gives 2,4,6-triamino-5-(4-nitrophenyl)pyrimidine (IV), m. 363-4° (hydrochloride m. 345-7°). III sealed 6 hrs. at 200° with 2N NaOH gives 2,4,6-triamino-5-(4-aminophenyl)pyrimidine, m. 230°, solidifies and m. 239°; hydrochloride m. 360°. I autoclaved 7 hrs. at 200° with piperidine, m. 346-7°. I (8 g.) autoclaved 7 hrs. at 200° with 24N cc. EtOH and 113 g. BuOH gives, on cooling, taking up the solid in CHCl3, and adding excess dry HCl in Et2O, a dihydrochloride which, on recrystn. from aq. gives a monohydrochloride of 2,4-di-amino-5-phenyl-6-dibutylaminopyrimidine, m. 104°. Similarly, I gives 2,4-diamino-5-(4-nitrophenyl)-6-dibutylaminopyrimidine, m. 171°.

IT 13175-56-3P, Hexamethylenimine, 1-(2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 13175-56-3 HCAPLUS
CN Hexamethylenimine, 1-(2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl)- (9CI) (CA INDEX NAME)

AN 1959:2101 HCAPLUS
DN 53:2101
OREF 53:390d-i,391a-f
TI Diuretics. Organomercurials. III. 4,6-Diaminopyrimidines
AU Whitehead, Calvert W.; Traverso, John J.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1958), 80, 2185-9
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
AB Dry 4-amino-6-hydroxypyrimidine (111.1 g.) and 1200 cc. POCl3 treated with stirring with 160 g. PhNEt2, refluxed 4.5 hrs., the excess POCl3 distilled at 50-5° in vacuo, the residual thick brown sirup dissolved in an equal volume of Et2O, cooled in Dry Ice-Me2CO, treated dropwise with stirring with 200 cc. cold H2O at -10 to 0° with the pH maintained at approx. 6 with NH4OH, stirred 2 hrs., warmed to room temperature, adjusted to pH 6, and extracted 2-2.5 days with Et2O, the extract evaporated, the residue washed with petr. ether, dissolved in about 4 l. hot H2O, treated with C, cooled, and the precipitate filtered off (concentration of the mother liquors gave addnl. product) yielded 70-90 g. 4-amino-6-chloropyrimidine (I), m. 215°. I (5 g.) in 100 cc. absolute EtOH saturated with cooling with dry HCl yielded 4 g. I HCl, m. 193° (decomposition) (EtOH). I (10 g.) and 0.14 mole appropriate alkylamine alone or in 50-100 cc. H2O, dioxane, EtOH, or PhMe refluxed 8-12 hrs. (low-boiling amines and I were heated at 110-20° in sealed tubes), cooled, filtered, concentrated, and the resulting precipitate recrystd. gave the corresponding 4-amino-6-(alkylamino)pyrimidines (II). I (10 g.) and 0.068 mole arylamine-HCl in 200 cc. dioxane and 30 cc. EtOH refluxed 24 hrs., cooled, the precipitate filtered off, dissolved in H2O, treated with C, the mixture filtered, basified with NH4OH, and the precipitated base recrystd. (aqueous EtOH) yielded the corresponding 4-amino-6-(substituted-amino)pyrimidines (III). By these procedures were prepared the following II and III (substituent on 6-amino group, % yield, m.p., and % diuretic activity given): Me, 62, 205°, 9, Et, 74, 193°, -; CH2:CHCH2, 65, 146°, 8, HO2C(CH2)2 (prepared by heating H2NCH2CH2CO2Na with I in H2O), 21, 225° (decomposition), -; Pr, 89, 140°, 15, iso-Pr, 81, 177°, 11; Bu, 78, 118°, 18 (pK'a 5.7), iso-Bu, 70, 125°, 16; furfuryl, 30, 172°, 11; Am, 72, 115°, 36, iso-Am, 50, 145°, 16; p-ClC6H4, 41, 179°, 40, Ph, 74, 179°, 100 (pK'a 4.9); 2-pyridylmethyl, 13, 188°, -, cyclohexyl, 54, 203°, 7; C6H13, 94, 115°, 11, m-MeC6H4, 35, 132°, 68, p-MeC6H4, 29, 175°, 100; PhCH2, 78, 211°, 69 (pK'a 5.0), p-MeOC6H4, 54, 215-20°, -; 1-hydroxycyclohexylmethyl, 70, 197°, - (pK'a 5.6); C7H15, 53, 119°, 16, o-ClC6H4CH2CH2, 47, 156°, -; Ph(CH2)2, 54, 164°, 13, MePhCH, 67, 171°, -; m-MeC6H4CH2, 94, 175°, 21, o-MeC6H4CH2, 90, 219°, -, p-MeC6H4CH2, 60, 206°, -, p-MeOC6H4CH2, 99, 131° (decomposition), -; PhO(CH2)2, 98, 190°, 86, 2-cyclohexylethyl, 60, 183°, -, C8H17, 76, 100°, -, 3,4-(CH2O2)C6H3(CH2)2, 55, 147°, -, Ph(CH2)3, 46, 107°, 38, p-MeOC6H4(CH2)2, 95, 165°, -; Ph(CH2)4, 98, 108°, -, 3,4-(MeO)2C6H3(CH2)2, 61, 152°, -, 3,4-(MeO)2C6H3(CH2)3, 45, 153°, -, PhC(C4H8)CH2, 48, 151°, -, Ph2CHCH2, 49, 143°, -. CH2[C(:NH)OEt]2 (23 g.) in 75 cc. absolute EtOH treated with 0.2 mole of the appropriate amine, the mixture shaken to solution, kept several days at room temperature, filtered, and the residue recrystd. (EtOH) yielded the corresponding CH2[C(:NH)NHR]22HCl (IV) (R, m.p. with decomposition, and % yield given): Et, 280°, 71; Bu, 290-5°, 49; CH2:CHCH2, 255°, 95; MeO(CH2)3, 230°, 59; C8H17, 280-90°, 78; furfuryl, 280°, 60; Ph(CH2)2, 300°, 61. The appropriate IV (0.05 mole) added with cooling to 5.4 g. NaOMe in 75 cc. EtOH, filtered, evaporated in vacuo, the residual sirup dissolved in 20 cc. HCO2Et, the solution kept 12 hrs. at room temperature, concentrated on the steam bath, cooled, and the crystalline deposit filtered off and recrystd. (50% EtOH) yielded the corresponding 4,6-bis(alkylamino)pyrimidines (alkyl group, % yield, m.p., and pK'a in 66% HCONMe2 given): Et, 79, 187°, 5.6; CH2:CHCH2, 19.5, 163°, 5.2; furfuryl, 14, 185°, 4.7; C8H17, 48, 112°, -. I (0.1 mole) treated in the usual manner with an appropriate secondary amine yielded the corresponding 4-amino-6-(substituted-amino)pyrimidines (6-substituent, % yield, and m.p. given): Me2N, 93, 202°;

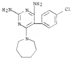
1-pyrrolidinyl, 95, 243°, Et2N, 39, 132° (pK'a 5.7), morpholino, 72, 197°, piperidino, 97, 185°, homopiperidino, 81, 208° (pK'a 5.7), Pr2N, 33, 99°, MePhN, 82, 181°. 4,6-Dichloropyrimidine (V) (7.4 g.) mixed with 21.5 g. PhCH2NH2, heated 3 hrs. on the steam bath, dissolved in hot EtOH, and cooled gave 6.5 g. 4,6-bis(benzylamino)pyrimidine, m. 234-5°, the filtrate evapd., and the residue recrystd. (EtOAc-petr. ether) yielded 2 g. 4-benzylamino-6-chloropyrimidine, m. 121°. V (6.7 g.) and 14.6 g. BuNH2 gave similarly 6.7 g. 4,6-bis(butylamino)pyrimidine (VI), m. 154°. PhO(CH2)2NH2 (6.85 g.) in 60 cc. 20% EtOH heated 12 hrs. on the steam bath with 3.95 g. V and cooled yielded 6 g. 4-chloro-6-(2-phenoxyethylamino)pyrimidine, m. 98-100° (EtOAc-petr. ether). Furfurylamine (5.9 g.) and 4.46 g. V in 50 cc. H2O heated several hrs. on the steam bath and cooled yielded 3.5 g. 4-chloro-6-(furfurylamino)pyrimidine, m. 130° (EtOAc-petr. ether). Similarly was prepd. 4-chloro-6-piperidino-pyrimidine, m. 78°, 93%. VI (1 g.) and 1 g. MeI in 25 cc. EtOAc refluxed 1 hr. and cooled gave 1.2 g. VI.MeI, m. 121°, pK'a in 66% HCONMe2 12.8. The pK'a values were detd. in 66% HCONMe2 for the following compds.: 4-amino-6-(-phenyl-1-cyclopentylamino)pyrimidine 5.5, 4-amino-6-(N-methylanilino)pyrimidine 5.0. The diuretic activities were detd. by comparing the increase in urine vol./kg. body wt. over the normal output during 3 hrs., starting 1 hr. after dosage, the diuretic response was from doses of 5 and 10 mg./kg., a value of 10% was obtained for a 20 mg./kg. dose of 1-allyl-3-ethyl-6-aminouracil. The LD50 values for the compds. tested varied between 500 and 1500 mg./kg. mice and rats.
IT 110378-52-4P, Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)-
RL: PREP (Preparation)
(preparation of)
RN 110378-52-4 HCAPLUS
CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



AN 1956:4978 HCAPLUS
DN 50:4978
OREF 50:1094d-i
TI Substituted 5-phenylpyrimidines
PA Societe des usines chimiques de Rhone-Poulenc
DT Patent
LA Unavailable
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI GB----712595		19540728	GB		<--

GI For diagram(s), see printed CA Issue.
AB Pyrimidines of amebicidal activity have been prepared at 150-200° (or higher) in an organic solvent by action of NH3 or primery and secondary amines on a pyrimidine derivative C(NH2):N.C(NHR):N.CY:CC6H3XX'-4,3, where X and X' may be H, Cl, MeO, NH2, NO2, or CN, Y is a halogen atom, and R is H or an acyl radical. (In the product Y is replaced by the corresponding primary, secondary, or tertiary amino radical, especially straight chain C1-5 alkyl, piperidino, hexamethyleneimino, or pyrrolidino groups.) Thus, 8 g. 2,4-diamino-5-(4-chlorophenyl)-6-chloropyrimidine, 16 ml. Bu2NH, and 50 ml. EtOH were heated in a stirred autoclave 7 hrs. at 200-210°; the cooled mixture was filtered, washed with H2O and EtOH, and the residue was recrystd. from aqueous EtOH to yield 2,4-diamino-5-(4-chlorophenyl)-6-dibutylaminopyrimidine (I), m. 116-17°. In the same way, using other amines, the following 6-substituted pyrimidines were prepared: Mc2N m. 212-13°, Et2N m. 208°, Pr2N m. 129-30°, BuNH m. 162-3°, piperidino m. 190°, hexamethyleneimino m. 153°, pyrrolidino m. 199-200°, A2N m. 140-50°; also from 2,4-diamino-5-(3,4-dichlorophenyl)-6-chloropyrimidine, the corresponding 6-Bu3N derivative, m. 106°. Heating 5 g. 2-acetamido-4,6-dichloro-5-(4-chlorophenyl)pyrimidine (II), 80 ml. absolute EtOH, and 40 g. liquid NH3 6 hrs. at 200° gave 2.4 g. 2,4,6-triamino-5-(4-chlorophenyl)pyrimidine, m. 280-1° (from EtOH). Also from 37 g. 2,4-diamino-5-phenyl-6-chloropyrimidine (III), 74 ml. EtOH, and 200 g. NH3 was obtained 21 g. 2,4,6-triamino derivative m. 241°, which was converted by action of KNO3 on a solution of the compound in concentrated H2SO4 at -15° to 2,4,6-triamino-5-(4-nitrophenyl)pyrimidine (IV), m. 362-5°; HCl salt, m. 302-5°. IV was reduced with PtO2 to the 5-(4-aminophenyl) analog, m. 220°, resolidifies, m. again at 238°, which was converted to the corresponding nitrile, m. 365-72°, by the Sandmeyer reaction. Also, 48 g. III, 150 ml. EtOH, and 113 g. Bu2NH at 200° for 7 hrs gave a residue which dissolved in CHCl3, from which a di-HCl salt was precipitated by HCl-Et2O addition which on recrystn. from H2O gave 2,4-diamino-5-phenyl-6-dibutylaminopyrimidine-HCl, m. 194°, which was nitrated to the 5-(4-nitrophenyl) compound, m. 171°. I was also prepared by heating 4 g. 2-amino-4-chloro-5-(4-chlorophenyl)-6-dibutylaminopyrimidine (V), 25 g. EtOH, and 24 g. NH3 6 hrs. at 200-10°. V, m. 147-8°, was made from II and excess Bu2NH at 110-15°.
IT 131975-96-7P, Hexamethylenlmine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]-
RL: PREP (Preparation)
(preparation of)
RN 131975-96-7 HCAPLUS
CN Hexamethylenimine, 1-[2,6-diamino-5-(p-chlorophenyl)-4-pyrimidinyl]- (6CI) (CA INDEX NAME)



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FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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FILE COVERS 1907 - 19 Feb 2008  VOL 148 ISS 8
FILE LAST UPDATED: 18 Feb 2008  (20080218/ED)

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L23 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2008 ACS on STN
AN 1966:93457 HCAPLUS
DN 64:93457
ORED 64.17589-a,17590-
TI Tetrazolo-4-alkoxomethine rearrangements in pyrimidine series
AU Szatkowski, Jozef; Zbirovsky, M. R.
CS Chem. Ustav Polytech. Inst., Hradec Kralove
SO Sbornik Vysokych Skol Chem. Technol. v Hradci Kralove, Oddeleni Organicke Technologie (1966), 1966(5), 113-34
CODEN: ZHKHAG; ISSN: 0300-3264
DT Journal
LA Russian
OS CASREACT 64:93457
AB Addition of NOBr, NOCl to 4,6-dialkoxypyrimidine in MeOH (exothermic) rapidly gave 4H4 4-hydroxino-6-chloropyrimidine, m. 144-5°, which boiled with aqueous amines 2 hr. gave 40-70% 6-hydroxino-4,6-substituted-pyrimidines (substituent shown): morpholino, m. 286-7°; N-homopiperidyl, m. 121-2°; piperidyl, m. 121-2°; and N-methylanilino, m. 121-2°. These treated with 2N HCl, followed by aqueous NaNO2 at 0°, gave 80-95% 4-azido-6-substituted-pyrimidines: morpholino, m. 91-3°, N-homopiperidyl, m. 93°. The remaining ones were converted by this reaction into tetrazolo[1,5-]-substituted-pyrimidines (I). Structures of the latter and their tautomeric open forms are shown. Thus, the presence of only electron-donor substituents leads to linear and cyclic nitrosation products. The tetrazole structures exists only in the solid state in the above products, in solution these were equilibrated with the azides (II), as shown spectroscopically
IT 5767-37-1P
(prepared from data in the 7th Collective Formula Index (1962-1966))
RN 5767-37-1 HCAPLUS
CN 1H-Azepine, 3-(6-azido-4-pyrimidinyl)hexahydro- (CA INDEX NAME)

IT 5767-37-1P, Hexamethyleneimine, 1-(6-hydrazino-4-pyrimidinyl)-
RL: PREP (Preparation)
(from data in the 7th Collective Formula Index (1962-1966))
RN 5767-37-1 HCAPLUS
CN 4(1H)-Pyrimidinone, 6-(hexahydro-1H-azepin-1-yl)-, hydrazone (8CI) (CA INDEX NAME)

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L1             1 US20070167459/PN

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L5                STR
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L8            50 L5 SAM SUB=L7
L9          2301 L5 FULL SUB=L7
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L22            2 L10

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L23            0 L10
L24            3 L9
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     FILE 'REGISTRY' ENTERED AT 17:28:18 ON 19 FEB 2008
L25            4 E63-66
L26            1 L25 AND C10H17N5

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L27            1 L26 AND L24

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FILE COVERS 1907 - 20 Feb 2008 VOL 148 ISS 8
FILE LAST UPDATED: 19 Feb 2008 (20080219/ED)

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substance identification.

=> d bib abs hitstr 111 tot

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2006:515480 HCAPLUS
DN 143:75535
TI Preparation of nitrogen-containing heterocyclic compounds as CXCR4 inhibitors
IN Watanabe, Tatsumi; Kohchi, Masaya; Shibayama, Shiro; Ieda, Hideaki; Kanzaki, Tetsuya
PA Eisai Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 441 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2006051963	A1	20060518	WO2005-JP19314	20051019
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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US20073674539	A1	20070719	US2005-5538758	20050410
PRAI JP2004-305148	A	20041020		
JP2004-362734	A	20041214		
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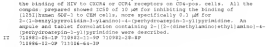
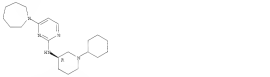


AB Compds. such as pyrimidine and quinazoline derivs. represented by the following general formulas (I) and (II), salts thereof, N-oxides thereof, solvates thereof or prodrugs of the same (wherein the ring A represents an optionally substituted nitrogen-containing heterocycle; the ring B represents an optionally substituted heterocycle; X represents a single bond, a heterocycle, Y represents an optionally substituted hydrocarbyl group, an optionally substituted heterocyclic group, an optionally protected amino group, an optionally protected hydroxyl group or an optionally protected mercapto group, and Z represents the ring A or an optionally substituted hydrocarbyl group) are provided. The compds. are useful as CXCR4 antagonists, and useful as preventives and/or remedies for various inflammatory diseases, immune diseases, various allergic diseases, infectious diseases, acquired immunodeficiency syndrome, infection with human immunodeficiency virus, psychiatric disorder, neurol. disease, cancer, tumor metastasis, osteoporosis, rheumatism, diabetes, cancer, and aspects for regeneration therapy, in particular transplant therapy. An assay system using SDF-1 which is an endogenous ligand of CXCR4 receptor, instead of HIV, was used in an assay for screening compds. which inhibit the binding of HIV to CXCR4 or CCR4 receptors on CD4-pos. cells. All the exemplified compds. of the present invention showed the binding of (125I)-human SDF-1 to CEM cells, more specifically 0.3 μM for 3-(1-benzylpyrrolidin-3-ylamino)-4-(pentyltetrahydro-3-yl)pyridine. An ampule and tablet formulation containing 2-((5-(dimethylaminomethyl)-amino)-4-(pentyltetrahydro-3-yl)pyridine were described.

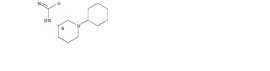
IT 711482-83-1P 711482-85-3P 711482-28-8P
711482-31-2P 711482-32-3P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)



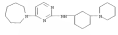
RN 711206-41-3 HCAPLUS
CN 4-Pyridinamine, N-(3R)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-3-yl)- (CA INDEX NAME)

Absolute stereochemistry



L11 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)
(Therapeutic use), BIOL (Biological study), PREP (Preparation); USES (Uses)
[prepn. of nitrogen-containg heterocyclic compds. as CXCR4 antagonists for treatment of diseases]

RN 711482-28-8 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-1H-azepin-3-yl)-N-[3-(1-piperidinylcyclohexyl- (CA INDEX NAME)



RN 710962-11-3 HCAPLUS
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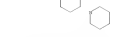
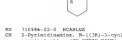
Relative stereochemistry



RN 710960-38-8 HCAPLUS
CN 3-Pyridinylamine, 4-(hexahydro-1H-azepin-3-yl)-N-[(3R,3R)-3-(1-piperidinylcyclohexyl)- rel- (CA INDEX NAME)

Relative stereochemistry.



RN 710958-62-0 HCAPLUS
CN 3-Pyridinylamine, N-[(3R)-1-cyclohexyl-3-piperidinyl]-4-(hexahydro-1H-azepin-3-yl)- (CA INDEX NAME)

Absolute stereochemistry.

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     (FILE 'HOME' ENTERED AT 13:08:43 ON 20 FEB 2008)

     FILE 'HCAPLUS' ENTERED AT 13:08:54 ON 20 FEB 2008
L1             1 US2007067459/PN

     FILE 'REGISTRY' ENTERED AT 13:09:18 ON 20 FEB 2008

     FILE 'HCAPLUS' ENTERED AT 13:09:18 ON 20 FEB 2008
L2             TRA L1 1- RN :     1829 TERMS

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L3          1829 SEA L2
                 ACT J758C4A/A
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L4               STR
L5   (      3911)SEA FILE=REGISTRY ABB=ON  PLU=ON  NC6/ES AND NCNC3/ES
L6          2301 SEA FILE=REGISTRY SUB=L5 SSS FUL L4
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L7          1368 L6 AND L3
L8            20 L6 AND O21H35N5
L9            12 L8 AND NC6/ES AND C6/ES AND NCNC3/ES
L10            5 L9 AND NC5/ES

     FILE 'HCAPLUS' ENTERED AT 13:13:11 ON 20 FEB 2008
L11            1 L10


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FILE 'HCAPLUS' ENTERED AT 13:32:23 ON 20 FEB 2008
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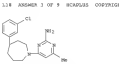
L14 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:124525/6 HCAPLUS
DN 144:150323
TI Preparation of pyrimidine derivatives as potential medicinal agents by the reaction of 1-amino-4-chloro-6-methylpyrimidine with primary and secondary amines
AU Ibrahim, Ismail
CS Department of Chemistry, Villanova University, Villanova, PA, 19085, USA
SO Journal of Heterocyclic Chemistry (2005), 42(7), 1295-1299
CODEN: JHTCAD; ISSN: 0120-5626
PB Heterocorporation
DT Journal
LA English
GA CASREACT 144:150323
AB Substituted derivs. of pyrimidine were prepared as potential medicinal agents by the reaction of 2-amino-4-chloro-6-(methyl)pyrimidine with primary and secondary amines. The reaction of 2-amino-4-chloro-6-methylpyrimidine (pirtetrazin)(pyrimidine derivs. the reagent prepared in this work may prove to be efficacious in the treatment of inflammation, hypertension, anxiety, depression, as anxiety (no biol. test data given).
IT 873829-86-6P
RL: PAC (Pharmacological activity); PREP (Preparation)
(preparation of pyrimidine derivs. via reaction of (alkoxychloromethyl)pyrimidine with primary and secondary amines)
RN 873829-86-6 HCAPLUS
CN 3-Pyridinamine, 4-(hexahydro-1H-azepin-1-yl)-6-methyl- (CA INDEX NAME)

RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1462059 HCAPLUS
DN 142:390365
TI Transformation of methyl N-methyl-N-(6-substituted-5-nitro-4-pyrimidinyl)aminoacetates into 4-methylamino-5-nitropyrimidines and pyrimido[4,5-b]azepines
AU Gavrilov, Yuriy; Brukstus, Algirdas; Tumkevicius, Eugijus
CS Department of Organic Chemistry, Faculty of Chemistry, Vilnius University, Vilnius, LT-03023, Lithuania
SO Tetrahedron Letters (2004), 46(33), 5613-5614
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 142:390365
GI

AB Upon treatment with sodium alkoxides, N-methyl-N-(6-amino-5-nitro-4-pyrimidinyl)aminoacetic acid Me esters [R1 = H, Ph, 3-FC6H4NH; R2 = H; R3 = Me, Et + MeOCOCH2; Ph; R1R2 = (CH2)4] undergo ring closure and rearrangement of nitrogen atom to afford 4-methylamino-5-nitropyrimidines II or 9-methylpurin-8-ones III depending on the nature of substituent in the 6 position of the pyrimidine ring.
IT 916013-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(transformation of methyl N-methyl-N-(6-substituted-5-nitro-4-pyrimidinyl)aminoacetates into 4-methylamino-5-nitropyrimidines and purinones by ring closure and rearrangement of nitrogen atom(s) in aminoacetates under basic conditions)
RN 916013-78-4 HCAPLUS
CN Glycine, N-(6-(hexahydro-1H-azepin-1-yl)-5-nitro-4-pyrimidinyl)-N-methyl-, methyl ester (CA INDEX NAME)



RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2004:123180 HCAPLUS
DN 140:324510
TI Preparation of substituted pyrimidines as active ingredients of novel antiallergic and insecticidal compositions
IN Lee, Hyung Gyun; Larsen, Martha Jane; Kobiak, Teresa Maria
PA USA
SO U.S. Pat. Appl. Pub., 16 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US2004034243	A1	20040219	2003US-0215033	20040805 <--
AU2004262923	A1	20050217	2004AU-0262923	20060706 <--
CA--2535975	A1	20050217	2004CA-2535975	20060706 <--
WO2005014573	A3	20050303	2004WO-US024892	20060706 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
EP--1654249	A1	20060510	2004EP-0761033	20060706 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
JP2007531781	T	20070315	2006JP-0523418	20060706 <--
PRAI 2003US-0492248P	P	20030801 <--
2004WO-US024892	W	20040706 <--

OS CASREACT 140:324510; MARPAT 140:324510
GI

AB The title compds. I [A, B = N, alkyl; non-substituted NH2, alkoxy; X = O, S, NH, NR; R = alkyl, OH, alkoxy, NH2, NHR, NR2; Y = O, S, NH, NR, CH2, CO2; when A and B are not both N, Y = CH, COR; R = H, alkyl, aralkyl] are effective in treating parasitic diseases, and for the prevention or treatment of parasites in a plant or agricultural crop, were prepared. Thus, reacting 4-chloro-2,6-diaminopyrimidine with 4-phenylpiperidine in the presence of Et3N in refluxing EtOH afforded 2,6-diamino-4-(4-phenylpiperidin-1-yl)pyrimidine. 0.9 M HCl in DMSO adjusted 4-(4-phenylpiperidin-1-yl)pyrimidine-2,6-diose hydrochloride which showed inhibited motility of the H. contortus larvae at 10 μM. The composition comprising the and to trees compds. T was also useful for preventing or treating parasitic diseases, is disclosed.
IT 873829-86-6P
RL: AGR (Agricultural use); BAC (Biological activity or effector); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted pyrimidines as active ingredients of novel antiallergic and insecticidal compns.)
RN 873829-86-6 HCAPLUS
CN 2-Pyrimidinamine, 4-(4-(3-methylphenyl)hexahydro-1H-azepin-1-yl)-6-methyl- (CA INDEX NAME)

L18 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN
AN 2005:1462059 HCAPLUS
DN 142:390365
TI Transformation of methyl N-methyl-N-(6-substituted-5-nitro-4-pyrimidinyl)aminoacetates into 4-methylamino-5-nitropyrimidines and pyrimido[4,5-b]azepines
AU Gavrilov, Yuriy; Brukstus, Algirdas; Tumkevicius, Eugijus
CS Department of Organic Chemistry, Faculty of Chemistry, Vilnius University, Vilnius, LT-03023, Lithuania
SO Tetrahedron Letters (2004), 46(33), 5613-5614
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier B.V.
DT Journal
LA English
OS CASREACT 142:390365
GI

AB Upon treatment with sodium alkoxides, N-methyl-N-(6-amino-5-nitro-4-pyrimidinyl)aminoacetic acid Me esters [R1 = H, Ph, 3-FC6H4NH; R2 = H; R3 = Me, Et + MeOCOCH2; Ph; R1R2 = (CH2)4] undergo ring closure and rearrangement of nitrogen atom to afford 4-methylamino-5-nitropyrimidines II or 9-methylpurin-8-ones III depending on the nature of substituent in the 6 position of the pyrimidine ring.
IT 916013-78-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(transformation of methyl N-methyl-N-(6-substituted-5-nitro-4-pyrimidinyl)aminoacetates into 4-methylamino-5-nitropyrimidines and purinones by ring closure and rearrangement of nitrogen atom(s) in aminoacetates under basic conditions)
RN 916013-78-4 HCAPLUS
CN Glycine, N-(6-(hexahydro-1H-azepin-1-yl)-5-nitro-4-pyrimidinyl)-N-methyl-, methyl ester (CA INDEX NAME)

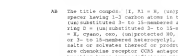
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2006 ACS on STN (Continued)

RN 841295-85-0 HCAPLUS
CN 2-Pyrimidinamine, 4-(hexahydro-4-methoxy-4-phenyl-1H-azepin-1-yl)-6-methyl- (CA INDEX NAME)

L14 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2024 ACS on STN
AN 2004:181666 HCAPLUS
DN 141196146
TI Preparation of nitrogen-containing heterocyclic derivatives as chemokine receptor CCR5 antagonists and drugs containing the same as the active ingredient
IN Imamura, Reona; Takaoka, Yoshiharu; Akahagawa, Shiro
PA Sumitomo Pharmaceutical Co., Ltd., Japan
SO PCT Int. Appl., 396 pp.
DOCBR: FCDOCS
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004018466	A2	20040304	WO2003-JP10333	20030813 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU2003257339	A1	20040309	AU2003-257339	20030813 <--
EP--1541549	A1	20050615	EP2003-788188	20030813 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
BR2003018731	A	20060131	BR2003-18731	20030813 <--
CN--1678996	A	20051005	CN 2004-80013005	20040312 <--
NO2005001354	A	20050314	NO2005-1354	20050313 <--
ZA2005017345	A	20060629	ZA2005-10734	20050913 <--
IN2005DN00948	A	20070413	IN2005-DN948	20050915 <--
KR2006178394	A	20061219	KR2005-7018126	20050915 <--
PRAI 2002JP-0270347	A	20020916 <--		
2003JP-0290412	A	20030731 <--		
2003WO-JP03333	A	20040312 <--		
OS MARPAT 141:196146				
GI				

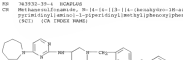


AB The title compds. [I; X1 = N, carboprotected acid group; X, Y = a bond, a spacer having 1-3 carbon atoms in the main chain; the ring A or B = (un)substituted 5- to 15-membered aromatic or heterocyclic ring; the ring D = (un substituted 3- to 15-membered N-containing heterocyclic ring; R2 = H, (un)substituted C1-6 alkyl, (un)substituted 3- to 15-membered ring or 3- to 15-membered heterocyclyl, -NCONR1 wherein R4 = H, C1-6 alkyl], salts or solvates thereof or prodrugs thereof are prepared. These compds. are conosidered receptor CCR5 antagonists and useful in preventing and/or treating human immunodeficiency virus (HIV) infection in particular, acquired immunodeficiency syndrome (AIDS), prevention of graft rejection in organ transplantation, and various inflammatory diseases (in particular, asthma. The various inflammatory diseases may also include sepsis, septicarpyaty, hepatitis, arthritis, rheumatoid arthritis, ylitis, conjunctivitis, and ulcerative colitis. The immunol. diseases may further include autoimmune diseases, psoriasis, and multiple sclerosis. They may be also useful for treating and/or preventing allergic diseases (atopic dermatitis, critisms, allergic bronchopulmonary

L14 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2024 ACS on STN (Continued)
aspergillosis, or allergic eosinophilic gastroenteritis), ischemic reperfusion injury, acute respiratory distress syndrome, and shock accompanying bacterial infections, diabetes, cancer metastases. Thus, a soln. of 1-[4-(methylsulfonyl)oxybenzoyl]piperidine-4-carboxamide, 744 mg N-tert-butoxycarbonyl-L-cyclohexylalanol, 0.140 mL n-butylamine, and 1.38 g HOBt in 20 mL dimethylformamide (I) was mixed at 45° for 12 h, treated with 5 mL conc. HCl, stirred for 2 h, concd., treated with 15 mL CHCl3 and 15 mL satd. aq. NaHCO3, and extd. twice with CHCl3 to give, after workup, a residue which was heated with 1.25 M AcOH/MeOH (2 mL) at 70° for 12 h to give, after workup and chromatog., 1-[4-(methylsulfonyl)oxybenzoyl]-N-[1-(n-butylcarbamoyl)-2-cyclohexylethyl]-4-diazoniopiperidine-2-ylpiperidin-4-yl]methylpiperidylbenzylmethanesulfonamide hydrochloride N-Bu(CyJ-H-[3-[4-[4-(methylsulfonyl)oxybenzoyl]piperidin-4-ylcarbonylaminocarbonyl]-2-cyclohexylethyl]-4-(pyridylmethyl)piperidine (II) inhibited the human monocyte chemotactic activity induced by human MCP-1 in a CHO cell study expressing receptor human CCR5 with IC50 of 0.677 μM. Pharmaceutical formulations, e.g. an ampule containing II were described.
IT 743932-39-4P 743932-39-4P
RL: SAC (Synthetic organic chemical); SPN (Synthetic preparation); TEM (Technical use); USES (Uses)
(preparation of nitrogen-containing heterocyclic derivs. as CCR5 antagonists for treating or preventing HIV infection, immune diseases, and inflammatory diseases)
RN 743932-39-4 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[4-[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)

● 3 HCl

RN 743932-39-4 HCAPLUS
CN Methanesulfonamide, N-[4-[4-[[4-[4-(hexahydro-1H-azepin-1-yl)-2-pyrimidinyl]amino]-1-piperidinyl]methyl]phenoxy]phenyl]-, trihydrochloride (9CI) (CA INDEX NAME)



● 3 HCl

IT 743933-71-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogen-containing heterocyclic derivs as CCR5 antagonists for

L14 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2024 ACS on STN (Continued)
treating or preventing HIV infection, immune diseases, and inflammatory diseases)
RN 743933-71-4 HCAPLUS
CN 3-Pyridinecarbox., 6-(hexahydro-1H-azepin-1-yl)-1-[6-(4-piperidinyl)-

● 3 HCl

RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2024 ACS on STN
AN 2004:183389 HCAPLUS
DN 141199700
TI Preventives and/or remedies for central diseases
IN Mizuguchi, Ayumi; Sasaki, Katsuhiro; Maejima, Koji, Aoyama, Shiro, Nosaka, Hiroki; Arai, Mitoshi, Shirokani, Akihiro; Kawase, Yoshihisa; Otsubo, Nobumasa
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 349 pp.
DOCBR: FCDOCS
DT Patent
LA Japanese
FAN.CNT 1

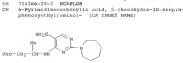
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004054613	A1	20040701	2003WO-JP15892	20031212 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU2003289338	A1	20040708	2003AU-AU289338	20031212 <--
PRAI 2002JP-0362104	A	20021213 <--		
2003WO-JP15892	W	20031212 <--		
OS MARPAT 141:99709				
GI				

AB It is intended to provide a preventive and/or a remedy for central diseases containing, as the active ingredient, a substance having an effect of inhibiting the activity of a protein kinase. Namely, a pyrimidine or pyridine derivative represented by the following general formula (I): X wherein A represents optionally substituted aryl, etc.; R1 represents hydrogen, etc.; R2 represents -NR3R4, etc.; X represents -CH= or -N=; and Y represents hydrogen, etc., its pharmacol. acceptable salt, etc
IT 743932-39-4P
RL: BAC (Biochemical activity); SPN (Synthetic preparation); TEM (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(G-protein coupled receptor 48-inhibiting pyrimidine derivs., pharmaceutical compns. containing them and preventives and/or remedies for central nervous system diseases)
RN 743932-39-4 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-(hexahydro-1H-azepin-1-yl)-4-[(3-methyl-2-phenoxyethyl)amino]- (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2024 ACS on STN (Continued)
AN 2004:183389 HCAPLUS
DN 141199700
TI Preventives and/or remedies for central diseases
IN Mizuguchi, Ayumi; Sasaki, Katsuhiro; Maejima, Koji, Aoyama, Shiro, Nosaka, Hiroki; Arai, Mitoshi, Shirokani, Akihiro; Kawase, Yoshihisa; Otsubo, Nobumasa
PA Kyowa Hakko Kogyo Co., Ltd., Japan
SO PCT Int. Appl., 349 pp.
DOCBR: FCDOCS
DT Patent
LA Japanese
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO2004054613	A1	20040701	2003WO-JP15892	20031212 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
AU2003289338	A1	20040708	2003AU-AU289338	20031212 <--
PRAI 2002JP-0362104	A	20021213 <--		
2003WO-JP15892	W	20031212 <--		
OS MARPAT 141:99709				
GI				



AB It is intended to provide a preventive and/or a remedy for central diseases containing, as the active ingredient, a substance having an effect of inhibiting the activity of a protein kinase. Namely, a pyrimidine or pyridine derivative represented by the following general formula (I): X wherein A represents optionally substituted aryl, etc.; R1 represents hydrogen, etc.; R2 represents -NR3R4, etc.; X represents -CH= or -N=; and Y represents hydrogen, etc., its pharmacol. acceptable salt, etc
IT 743932-39-4P
RL: BAC (Biochemical activity); SPN (Synthetic preparation); TEM (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(G-protein coupled receptor 48-inhibiting pyrimidine derivs., pharmaceutical compns. containing them and preventives and/or remedies for central nervous system diseases)
RN 743932-39-4 HCAPLUS
CN 3-Pyridinecarboxylic acid, 2-(hexahydro-1H-azepin-1-yl)-4-[(3-methyl-2-phenoxyethyl)amino]- (CA INDEX NAME)

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:83166 HCAPLUS
DN 68:83166
OREF 68:16972a-d
TI Resolution of several racemic barbitals into optical antipodes. III. Barbituric acid derivatives
AU Shabe, J.; Phillipson, E
CS Tech. Hochsch., Braunschvelg, Germany
SO Arzneim.-Forsch. (1968), 18(1), 323-42
DT Journal
LA German
CC CAPPLECT 66:93436
GI For diagram(s), see printed CA Issue
AB Cf. CA 66, 93436. The 5-(1-methylbutyl) (I; R = Et, R' = Me; II; R = Pr, R' = Me; III; R = Me-Pr, R' = CH2:CHCH2, R'' = Me) (III) was achieved through the N-methylbrucinium salts. This method is also suitable for the resolution of N-unsubstituted barbitals with an asym. center in a C-5 side chain as demonstrated on the examples pentobarbital and vinylbital. II (R = Et, R' = Me) (0.1 mole) and 0.1 mole brucine (IV) in 1 l. 95% EtOH/ 2 diastereomeric II-IV salts. III (0 81 g.) dissolved in 145.0 cc. MeOH containing 1 equivalent IV, concentrated to 1/3 volume and diluted with H2O to turbidity gave 5.8 g. (+)-IV, m. 214° (MeOH-H2O); the mother liquor diluted with H2O gave 5.8 g. mixture and then 4.5 g. (-)-IV, m. 136° (MeOH-H2O). (+)-IV (5.8 g.) in 100 cc. MeOH and H2O yielded 3.8 g. (+)-II, m. 161°, α]D 3.84° (c 2.19, absolute EtOH). (-)-II-IV (6.5 g.) gave similarly 1.2 g. (-)-II, m. 161°, α]D -3.92° (c 2.74, absolute EtOH). III (11.33 g.) in 145.0 cc. MeOH containing 1 equivalent IV yielded 8.9 g. (+)-III-IV, m. 128° (MeOH-H2O); liberated 3 cc. 2N NaOH and 3.7 g. (+)-III, α]D 7.5° (c 1.77, 95% EtOH). (-)-III-IV, m. 128° (MeOH-H2O), liberated 3 cc. 2N NaOH and 3.7 g. (-)-III, α]D -7.5° (c 1.77, 95% EtOH). (+)-III (5.9 g.) yielded similarly 1.0 g. (+)-III, m. 150°, α]D +2.92° (c 0.932, absolute EtOH). I (R = Et, R' = MeCH2CH, R'' = H) (V) with IV yielded 5.2 g. (+)-V-IV, m. 210° (MeOH-H2O); 31.2 g. mixture, and 4.2 g. (-)-V-IV, m. 128° (MeOH-H2O). (+)-V-IV (5.2 g.) yielded similarly 1.5 g. (+)-V, m. 158°, α]D +2.19° (c 1.82, absolute EtOH). (-)-V-IV (4.2 g.) in MeOH with NH4OH yielded 1.1 g. (-)-V, m. 84°, α]D -0.46° (c 4.79, absolute EtOH). (+)-VI-IV gave similarly 2.8 g. (+)-VI, m. 84°, α]D 0.39° (c 3.46, absolute EtOH). The ir spectra of (+)-II and (+)-III were recorded.
IT 57-43-2
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 4764-10-6 HCAPLUS
CN 1H-Azepine, 1-(6-azido-4-pyridinyl)hexahydro- (CA INDEX NAME)

L18 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:13100 HCAPLUS
DN 63:23192
OREF 63:4196a-f,4197a-d
TI Diversion. Organomercurials. II. Alkoxymercuration by mixed anion salts of mercury
AU Whitehead, Calvert W.; Traverso, John J.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1968), 89, 2182-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
CC CAPPLECT 53:2100
GI For diagram(s), see printed CA Issue
AB Hg(OAc)2 (0.1M-1.0 g.) and an equimolar amount of MgCl2, MgBr2, MgI2, Mg(NO3)2, or Mg(AcO)2 were added to the appropriate alc. reactant or MeOH; the resulting mixed mercuric salts were treated, without isolation, with the allylanides. The appropriate alkene-sulfonyl chloride added dropwise with stirring to 1 g. CH2:CHCH2NH2 in 500 cc. MeOH, 1 g. Et3N, and 1 g. mole equivalent CH2Cl2, and the Et3N solution washed after 1 hr. with H2O, dried, and evaporated gave the corresponding amides; in the preparation of the N-O-acetoxy-N-Me deriv., the Et3N solution was cooled and the CH2Cl2 filtered off. in this manner were prepared the following RSO2NR'CH2CH:CH2 (I) (R, R', m.p., °C., and %): Me, H, 59-60°, 60; Me, Me, oil, 70; Me, Ac, (II), 83°/0.5, 43; Et, H, 51-2°/0.5, 70; Et, Me, oil (III), 114°/1.5, 48; Et, Ac, (IV), 110°/0.5, 30. The appropriate N,N-dialkylsulfamoyl chloride (0.5 mole) added dropwise with stirring to 57 g. CH2:CHCH2NH2 in 500 cc. Et2O, and the mixture washed with H2O, dried, and concentrated gave the following RR'NSO2NHCH2CH:CH2 (V): R, R', b.p./mm., and % yield given: Me2N, 110°/0.1, 76; Et2N, 102°/0.1, 62; pyrrolidino, 140°/0.7, 92; morpholino, ~ 1m. 140°), 68; Et2N, 114°/1.0, 44. The appropriate I (0.2 mole) and 0.2 mole AcONgCl in 200 cc. H2O or AcOHgOe in MeCOO warmed on the steam bath to about 40°, kept 1 hr. at room temperature, and filtered gave the corresponding RNHCHCH(OR')CH2HgX (VI) (R, R', X, m.p., and % yield given): Me, Me, Cl, 115°, 90; Me, Me, AcO, 110°, 90; Et, Me, Cl, 84°, 92; t-Bu(gal)Lucas(ligal, Me, Cl (VI), 118°, 32. The products from II, III, and IV were oily and could not be characterized; the products from the I (R = dialkylamino) were sirups or plastics. CH2:CHCHNSO2 (236 cc.) and 132 g. NCHCOHNSCOOMe refluxed 2(hr. with stirring, concentrated in vacuo, and the residue extracted 10 g. NCHOOHNSCOOMeCOOH CH2 (VII), m. 167-8° VII (15.7 g.) stirred with 0 l mole AcONgCl in 200 cc. MeOH, AcOHgOe in 100 cc. MeOH, AcOHgCl in 500 cc. MeOH, and AcOHgCl in 200 cc. H2O, kept 12 hr. at room temperature, filtered, and each product reoxyrtd. (MeOH) gave the following V (R = dialkylamino, R', X, m.p., °C., and % yield given): Me2N, H, Cl, decomposition), 62. Me, Me, Cl, 171° (decomposition), 90; Me, AcO (), 132° (decomposition), 40. RSCHNCHCHNCHCOH CH2 (9 g.) added to 0.2l6 mole AcONgCl in 25 cc. MeOH (and in 75 cc. MeOH), kept 2-5 days at room temperature, filtered, and the filtrate concentrated in vacuo gave VIII (R = dialkylamino): H, H, m.p., and % yield given: H, Cl (IX), 84°, 94. Me, Cl (IX), 91°, 96. 3-Allyl-5-carbothorpyrazil (VIII) (23.4 g.) and 155 cc. 1 2N NaOH treated dropwise with stirring at 10° with 12.6 g. MeCl2O, concentrated in vacuo, cooled, and the residue recrystd. (EtAlo-pur) gave 3-allyl-5-carbothorpyrazil-1-carbothoic acid (X), m. 140-1°. X (2 g.) By(OAc)2, and 4 g. XIV in 50 cc. MeOH heated 5 min. on the steam bath, filtered, and cooled gave 7.8 g. 3-ClHgCH2CH(OMe)CH2 analog (XV) of XIV, m. 146° (MeOH). Hg(AcO)2 (2.0 g.) in 5 m.f Mg(NO3)2, 1.4 g XIV, and 50 cc. MeOH warmed 5 MIN. at 50-60°, filtered, and cooled gave 3.2 g. 3-ClHgCH2CH(OMe)CH2 analog (XVI), m. 140°. 1,3-Diallyl-5-carbothorpyrazil (XVII), 2000 cc. Alcohol, and 40 cc. CH2:CHCH2NH2 heated overnight at 110° in a bomb, evaporated in vacuo, the residue dissolved in the min. amount of H2O, the aqueous solution treated with C, cooled, and the precipitate crystallized from a bomb volume of H2O yielded 41 g. 1,3-Diallyl-5-(N-allylcarbothoryl) (XVIII), needles, 207°. 1,3-Diallyl-5-carbothorpyrazil (XVII), 2000 cc. Alcohol, and 150 cc ETI (1) g.) heated to boiling with 0.95 mole NaOH in 150 cc. MeOH, concentrated in vacuo, cooled, and the residue in 2000 cc. MeOH, AcONgCl in 150 cc. MeOH, AcONgCl in 150 cc. MeOH, AcONgCl in 150 cc. MeOH, AcOHgCl in 150 cc. MeOH, AcOHgCl in 60 cc. MeOCH2CH2OH, cooled, kept at room temperature, filtered, and the residue recrystd. (CHCl3-I) yielded the following compds. (XVIII) (R, X, m.p., and % yield given): H, Cl (XIX), 154°, 90; Me, Cl (XIX), 154°, 90; Me, AcO (XIX), 215°, 42; Me, I (XIX), 183°, 95; Me, AcO- (XIX), 116-7°, 70, Et, Cl, (XIX), (XVIII) 170-98°, 83; MeO(CH2)2O,

L18 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1968:83166 HCAPLUS
DN 68:83166
OREF 68:16972a-d
TI Resolution of several racemic barbitals into optical antipodes. III. Barbituric acid derivatives
AU Shabe, J.; Phillipson, E
CS Tech. Hochsch., Braunschvelg, Germany
SO Arzneim.-Forsch. (1968), 18(1), 323-42
DT Journal
LA German
CC CAPPLECT 66:93436
GI For diagram(s), see printed CA Issue
AB Cf. CA 66, 93436. The 5-(1-methylbutyl) (I; R = Et, R' = Me; II; R = Pr, R' = Me; III; R = Me-Pr, R' = CH2:CHCH2, R'' = Me) (III) was achieved through the N-methylbrucinium salts. This method is also suitable for the resolution of N-unsubstituted barbitals with an asym. center in a C-5 side chain as demonstrated on the examples pentobarbital and vinylbital. II (R = Et, R' = Me) (0.1 mole) and 0.1 mole brucine (IV) in 1 l. 95% EtOH/ 2 diastereomeric II-IV salts. III (0 81 g.) dissolved in 145.0 cc. MeOH containing 1 equivalent IV, concentrated to 1/3 volume and diluted with H2O to turbidity gave 5.8 g. (+)-IV, m. 214° (MeOH-H2O); the mother liquor diluted with H2O gave 5.8 g. mixture and then 4.5 g. (-)-IV, m. 136° (MeOH-H2O). (+)-IV (5.8 g.) in 100 cc. MeOH and H2O yielded 3.8 g. (+)-II, m. 161°, α]D 3.84° (c 2.19, absolute EtOH). (-)-II-IV (6.5 g.) gave similarly 1.2 g. (-)-II, m. 161°, α]D -3.92° (c 2.74, absolute EtOH). III (11.33 g.) in 145.0 cc. MeOH containing 1 equivalent IV yielded 8.9 g. (+)-III-IV, m. 128° (MeOH-H2O); liberated 3 cc. 2N NaOH and 3.7 g. (+)-III, α]D 7.5° (c 1.77, 95% EtOH). (-)-III-IV, m. 128° (MeOH-H2O), liberated 3 cc. 2N NaOH and 3.7 g. (-)-III, α]D -7.5° (c 1.77, 95% EtOH). (+)-III (5.9 g.) yielded similarly 1.0 g. (+)-III, m. 150°, α]D +2.92° (c 0.932, absolute EtOH). I (R = Et, R' = MeCH2CH, R'' = H) (V) with IV yielded 5.2 g. (+)-V-IV, m. 210° (MeOH-H2O); 31.2 g. mixture, and 4.2 g. (-)-V-IV, m. 128° (MeOH-H2O). (+)-V-IV (5.2 g.) yielded similarly 1.5 g. (+)-V, m. 158°, α]D +2.19° (c 1.82, absolute EtOH). (-)-V-IV (4.2 g.) in MeOH with NH4OH yielded 1.1 g. (-)-V, m. 84°, α]D -0.46° (c 4.79, absolute EtOH). (+)-VI-IV gave similarly 2.8 g. (+)-VI, m. 84°, α]D 0.39° (c 3.46, absolute EtOH). The ir spectra of (+)-II and (+)-III were recorded.
IT 57-43-2
(Derived from data in the 7th Collective Formula Index (1962-1966))
RN 4764-10-6 HCAPLUS
CN 1H-Azepine, 1-(6-azido-4-pyridinyl)hexahydro- (CA INDEX NAME)

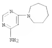
L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2004 ACS on STN
AN 1969:13100 HCAPLUS
DN 63:23192
OREF 63:4196a-f,4197a-d
TI Diversion. Organomercurials. II. Alkoxymercuration by mixed anion salts of mercury
AU Whitehead, Calvert W.; Traverso, John J.
CS Lilly Research Labs., Indianapolis, IN
SO Journal of the American Chemical Society (1968), 89, 2182-6
CODEN: JACSAT; ISSN: 0002-7863
DT Journal
LA Unavailable
CC CAPPLECT 53:2100
GI For diagram(s), see printed CA Issue
AB Hg(OAc)2 (0.1M-1.0 g.) and an equimolar amount of MgCl2, MgBr2, MgI2, Mg(NO3)2, or Mg(AcO)2 were added to the appropriate alc. reactant or MeOH; the resulting mixed mercuric salts were treated, without isolation, with the allylanides. The appropriate alkene-sulfonyl chloride added dropwise with stirring to 1 g. CH2:CHCH2NH2 in 500 cc. MeOH, 1 g. Et3N, and 1 g. mole equivalent CH2Cl2, and the Et3N solution washed after 1 hr. with H2O, dried, and evaporated gave the corresponding amides; in the preparation of the N-O-acetoxy-N-Me deriv., the Et3N solution was cooled and the CH2Cl2 filtered off. in this manner were prepared the following RSO2NR'CH2CH:CH2 (I) (R, R', m.p., °C., and %): Me, H, 59-60°, 60; Me, Me, oil, 70; Me, Ac, (II), 83°/0.5, 43; Et, H, 51-2°/0.5, 70; Et, Me, oil (III), 114°/1.5, 48; Et, Ac, (IV), 110°/0.5, 30. The appropriate N,N-dialkylsulfamoyl chloride (0.5 mole) added dropwise with stirring to 57 g. CH2:CHCH2NH2 in 500 cc. Et2O, and the mixture washed with H2O, dried, and concentrated gave the following RR'NSO2NHCH2CH:CH2 (V): R, R', b.p./mm., and % yield given: Me2N, 110°/0.1, 76; Et2N, 102°/0.1, 62; pyrrolidino, 140°/0.7, 92; morpholino, ~ 1m. 140°), 68; Et2N, 114°/1.0, 44. The appropriate I (0.2 mole) and 0.2 mole AcONgCl in 200 cc. H2O or AcOHgOe in MeCOO warmed on the steam bath to about 40°, kept 1 hr. at room temperature, and filtered gave the corresponding RNHCHCH(OR')CH2HgX (VI) (R, R', X, m.p., and % yield given): Me, Me, Cl, 115°, 90; Me, Me, AcO, 110°, 90; Et, Me, Cl, 84°, 92; t-Bu(gal)Lucas(ligal, Me, Cl (VI), 118°, 32. The products from II, III, and IV were oily and could not be characterized; the products from the I (R = dialkylamino) were sirups or plastics. CH2:CHCHNSO2 (236 cc.) and 132 g. NCHCOHNSCOOMe refluxed 2(hr. with stirring, concentrated in vacuo, and the residue extracted 10 g. NCHOOHNSCOOMeCOOH CH2 (VII), m. 167-8° VII (15.7 g.) stirred with 0 l mole AcONgCl in 200 cc. MeOH, AcOHgOe in 100 cc. MeOH, AcOHgCl in 500 cc. MeOH, and AcOHgCl in 200 cc. H2O, kept 12 hr. at room temperature, filtered, and each product reoxyrtd. (MeOH) gave the following V (R = dialkylamino, R', X, m.p., °C., and % yield given): Me2N, H, Cl, decomposition), 62. Me, Me, Cl, 171° (decomposition), 90; Me, AcO (), 132° (decomposition), 40. RSCHNCHCHNCHCOH CH2 (9 g.) added to 0.2l6 mole AcONgCl in 25 cc. MeOH (and in 75 cc. MeOH), kept 2-5 days at room temperature, filtered, and the filtrate concentrated in vacuo gave VIII (R = dialkylamino): H, H, m.p., and % yield given: H, Cl (IX), 84°, 94. Me, Cl (IX), 91°, 96. 3-Allyl-5-carbothorpyrazil (VIII) (23.4 g.) and 155 cc. 1 2N NaOH treated dropwise with stirring at 10° with 12.6 g. MeCl2O, concentrated in vacuo, cooled, and the residue recrystd. (EtAlo-pur) gave 3-allyl-5-carbothorpyrazil-1-carbothoic acid (X), m. 140-1°. X (2 g.) By(OAc)2, and 4 g. XIV in 50 cc. MeOH heated 5 min. on the steam bath, filtered, and cooled gave 7.8 g. 3-ClHgCH2CH(OMe)CH2 analog (XV) of XIV, m. 146° (MeOH). Hg(AcO)2 (2.0 g.) in 5 m.f Mg(NO3)2, 1.4 g XIV, and 50 cc. MeOH warmed 5 MIN. at 50-60°, filtered, and cooled gave 3.2 g. 3-ClHgCH2CH(OMe)CH2 analog (XVI), m. 140°. 1,3-Diallyl-5-carbothorpyrazil (XVII), 2000 cc. Alcohol, and 40 cc. CH2:CHCH2NH2 heated overnight at 110° in a bomb, evaporated in vacuo, the residue dissolved in the min. amount of H2O, the aqueous solution treated with C, cooled, and the precipitate crystallized from a bomb volume of H2O yielded 41 g. 1,3-Diallyl-5-(N-allylcarbothoryl) (XVIII), needles, 207°. 1,3-Diallyl-5-carbothorpyrazil (XVII), 2000 cc. Alcohol, and 150 cc ETI (1) g.) heated to boiling with 0.95 mole NaOH in 150 cc. MeOH, concentrated in vacuo, cooled, and the residue in 2000 cc. MeOH, AcONgCl in 150 cc. MeOH, AcONgCl in 150 cc. MeOH, AcONgCl in 150 cc. MeOH, AcOHgCl in 150 cc. MeOH, AcOHgCl in 60 cc. MeOCH2CH2OH, cooled, kept at room temperature, filtered, and the residue recrystd. (CHCl3-I) yielded the following compds. (XVIII) (R, X, m.p., and % yield given): H, Cl (XIX), 154°, 90; Me, Cl (XIX), 154°, 90; Me, AcO (XIX), 215°, 42; Me, I (XIX), 183°, 95; Me, AcO- (XIX), 116-7°, 70, Et, Cl, (XIX), (XVIII) 170-98°, 83; MeO(CH2)2O,

L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
Cl (XXV), 154°, 90. The apparent equil. consts. for the reaction RHgX + OH- dblarw RHgOH + X- at half-conversion were detd. in 66% HCONMe2 (the values in parentheses were detd. in H2O) for the following compds. (equil. const. given): IX, 2.1 + 103 (640); X, 7 + 105 (2.6-2.7 + 103); XI, 1.5 + 104 (1.4 + 104); XII, 0.9 + 104; XIX, 1.2 + 104 (1.0 + 104); XX, 1.1 + 103; XXI, 6.4 + 103; XXII, 47; XXIII, 2.3 + 105; XXIV, 8.1 + 103; XXV, 8.1 + 103; XV, 1.1 + 104 (0.9 104), XVI, 3.2 + 105; H2NCONHCH2CH(OMe)CH2HgI (XXVI), 130. XXVI, m. 165°, was prepd. in the standard manner in 70% yield.

IT 110378-52-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 110378-52-4 HCAPLUS

CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



L18 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN

AN 1959:2099 HCAPLUS

DN 53:2099

OREF 53:387h-i,388a-i,389a-c

TI Diuretics. Organomercurials

AU Whitehead, Calvert W.

CS Lilly Research Labs., Indianapolis, IN

SO Journal of the American Chemical Society (1958), 80, 2178-82
CODEN: JACSAT; ISSN: 0002-7863

DT Journal

LA Unavailable

OS CASREACT 53:2099

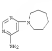
AB The appropriate HOC6H4CO2Me (152 g.) and 124 g. CH2:CHCH2NH2 heated 12 hrs. in a sealed tube at 100-30°, cooled, diluted with cold H2O, acidified with HCl, extracted with Et2O, and the extract worked up gave the corresponding crude HOC6H4CONHCH2CH:CH2 (I) (position of OH group, m.p., and % yield given): m, 87°, 89; o, - (oil), 71, p, -, 80. The appropriate crude I (42 g.) and 26.5 g. ClCH2CO2H refluxed 2 hrs. with 34 g. NaOH in 2 l. H2O, treated again with 26.5 g. ClCH2CO2H and 17 g. NaOH, refluxed 1.5 hrs., cooled, and acidified with concentrated HCl, and the precipitate recrystd. (EtOH) gave the corresponding HO2CCH2OC6H4CONHCH2CH:CH2 (II) (position of HO2CCH2O group, % yield, and m.p. given): m, 99, 120°, p, 44, 139°; o, 70, 121.5°. o-II (23.5 g.) and 100-300 cc. appropriate alcohol treated with stirring with 21.6 g. red HgO, heated 2-4 hrs. at 60°, filtered warm, the filtrate cooled, and the crystalline deposit recrystd. (EtOH or EtOH-HCONMe2) yielded the corresponding anhydro-o-[N-(3-hydroxymercuri)-2-(2-alkoxypropyl)carbamoyl)]phenoxyacetic acid (alkoxy group, m.p., and % yield given): HO(CH2)2O (III), - (decomposition), 80, MeO(CH2)2O (IV), 135°, 52; BuO, 171°, 90, EtO(CH2)2O, 139°, 54, HO(CH2)2O(CH2)2O, 162°, 55, BuO(CH2)2O, 133°, 70; PhO(CH2)2O, 197°, 88; Et2CHCH2O(CH2)2O, 124°, 70; C10H21O, 164°, 39. In the preparation of IV the product was obtained as the MeO(CH2)2OH (V) solvate, m. 75°, which, recrystd. (EtOH) gave IV. m-II (4.8 g.), 6.4 g. Hg(OAc)2 (VI), and 25 cc. V allowed to stand 3 days, diluted with petr. ether, filtered, and the residue washed with EtOH and then Et2O yielded 7 g. m-isomer of IV; it did not have an identifying m.p. m-II (4.8 g.), 6.4 g. VI, and 25 cc. (CH2OH)2 allowed to stand 3 days diluted with H2O, and the gummy precipitate triturated with EtOH and with Et2O yielded 7.5 g. amorphous m-isomer of III. p-II (4.8 g.), 6.4 g. VI, and 40 cc. (CH2OH)2 gave 7 g. p-{N-[3-acetoxymercuri-2-(2-hydroxyethoxy)propyl]carbamoyl}phenoxyacetic acid, m. 145° (ETOH). Dry BuOH (75 cc.), 5.2 g. 2-nonenoic acid, and 10.6 g. VI stirred until dissolved, allowed to stand a few hrs., filtered, and the residue washed with hot MeOH yielded 10 g. anhydro-3-butoxy-2-(hydroxymercuri)nonanoic acid, m. 186-8° (decomposition). Ph(CH2)2CH:CHCO2H (8.8 g.) in 50 cc. MeOH and 15.9 g. VI stirred to solution, kept 0.5 hr. at room temperature, filtered, and the residue washed with MeOH yielded 15 g. anhydro-2-hydroxymercuri-3-methoxy-5-phenylpentanoic acid, m. 189-90°. p-HOC6H4CH2CO2Et (97 g.) and 45 g. CH2.CHCH2NH2 refluxed 24 hrs., evaporated in vacuo, the residual sirup dissolved in the min. amount of warm EtOAc, and the solution diluted with petr. ether to incipient turbidity yielded 86 g. p-HOC6H4CH2CONHCH2CH:CH2 (VII), m. 84° [(CH2Cl)2]. VII (0.1 mole) treated with 18.8 g. ClCH2CO2H in aqueous NaOH yielded 29 g. p-HO2CCH2OC6H4CH2CONHCH2CH:CH2 (VIII), m. 137-9°. VII (50 g.), 32 g. ClCH2CO2Et, and 71 g. K2CO3 in 500 cc. Me2CO refluxed 48 hrs., evaporated, and the residual sirup crystallized from EtOAc and petr. ether yielded 51 g. Et ester of VIII, m. 86°. m-I (48 g.), 44 g. ClCH2CO2Et, and 50 g. K2CO3 in 300 cc. Me2CO yielded 40 g. Et ester of m-II, b1 204°. p-II (89 g.) in 1 l. absolute EtOH refluxed 12 hrs. with 30 cc. concentrated H2SO4, evaporated in vacuo, and the residue poured onto 1 kg. ice and filtered yielded 83 g. Et ester of p-II, m. 104-5° (EtOAc-petr. ether). The Et ester of o-II, m. 78°, was prepared similarly in 80% yield. p-HSC6H4SO3H (128 g.) and 64.6 g. ClCH2CO2H heated several hrs. on the steam bath with 81 g. NaOH in 500 cc. H2O, cooled, and filtered gave 266 g. di-Na salt of p-HO3SC6H4SCH2CO2H, the salt kept 24 hrs. with POCl3 at room temperature, refluxed 2 hrs., evaporated in vacuo, and the residual oil stirred 1 hr. with cold H2O yielded 106 g. p-ClO2SC6H4CH2CO2H, a 26.6-g. portion with 5.7 g. CH2:CHCH2NH2 gave 16 g. p-CH2:CHCH2NHO2SC6H4SCH2CO2H, m. 129-30°. p-CH2:CHCH2OC6H4CO2H (17.8 g.) in 75 cc. of the appropriate alc. allowed to stand at room temperature with

L18 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2008 ACS on STN (Continued)
31.8 g. VI and the ppt. washed with H2O, Et2O, and Et2O gave the corresponding p-(3-hydroxymercuri-2-alkoxypropoxy)benzoic acids (alkoxy group and % yield given): MeO, 68; HO(CH2)2O, 73; both acids decompd. on heating. p-H2NC6H4CH2CO2H (10.5 g.) and 8.3 g. MeCH:CHCOCl in aq. NaHCO3 yielded 9 g. p-MeCH:CHCONHC6H4CH2CO2H (IX), m. 206°. Similarly was prepd. p-MeCH:CHCONHC6H4CO2H, m. 268°, 70%. IX (1 g.), 1.5 g. VI, and 15 cc. (CH2OH)2 allowed to stand 5 days yielded 2 g. p-[2-(2-hydroxyethoxy)-3-(hydroxymercuri)butyrylamino]phenylacetic acid, m. 205° (decompn.). N-Allyl-N'-succinylurea (20 g.) in 40 cc. (CH2OH)2 treated with stirring with 32 g. VI, kept 2 days at room temp., distd. at 120°/0.1 mm., the sirupy residue dissolved in MeOH, treated with C, filtered, dild. with Et2O, the pptd. oil dissolved in the min. amt. of H2O, and the soln. adjusted with aq. NaOH to pH 7.5 and evapd. in vacuo yielded 60% N-[3-hydroxymercuri-2-(2-hydroxyethoxy)propyl)-N'-succinylurea Na salt. VI (6.4 g.) and 0.02 mole unsatd. compd. in 10-25 cc. of the appropriate alc. or 25 cc. H2O kept 2-5 days at room temp., filtered, and the residue recrystd. (EtOAc or EtOAc-petr. ether) gave the following p-EtO2CC6H4OCH2CH(OR)CH2HgOAc (R, m.p., and % yield given): Me, 78°, 70, Et, 76°, 75, MeO(CH2)2, 52°, 78. The following EtO2CCH2OC6H4CONHCH2-CH(OR)CH2HgOX were prepd. (position of substituents on the benzene nucleus, R, X, m.p., and % yield given): o, Cl(CH2)2, H, 145°, 98; p, H, Ac (hydrate), 149°, 60, o, MeO(CH2)2, Ac, 107°, 67; p, EtO2CMeCH, H, 110°, 55; o, EtO(CH2)2, Ac, 142°, 75; o, BuO(CH2)2, Ac, 145°, 70. Similarly were prepd. the following compds. (g. yield, and m.p. given): N-[3-acetoxymercuri-2-(2-methoxyethoxy)propyl]phthalimide(X), 9, 109°; 2-(2-hydroxymethoxy)propyl analog of X, 9.5, 126°; AcOHgCH2CH(OCH2CH2OH)CH2C(OH)Ph2, 4.5, 114.5°; AcOHgCH2CH(OMe)CH2C(OH)PH2 7.2, 135.6-36°; HO(CH2)2OCHPhCH(HgOH)CO2Me, 6.9, 216-18° (decompn.); MeO(CH2)2OCHPhCH(HgOAc)CO2Me, 7.9, 97°; Cl(CH2)OCHPhCH(HgOAc)2CO2Me, 7.5, 124°. 4,3-HO(CH2:CHCH2)C6H3CO2Et (2 g.) and 3.18 g. VI in 5 cc. (CH2OH)2 kept 3 days at room temp., dild. with Et2O, and filtered gave 4 g. 4,3-HO[AcOHgCH2CH(OCH2CH2OH)CH2]C6H3CO2Et, m. 99-100° (EtOAc-petr. ether). Similarly was prepd. in MeOH 4,3-HO[AcOHgCH2CH(OMe)CH2]C6H3CO2Et, m. 124-5°, 50%. In similar runs with EtOH, MeO(CH2)2OH, or PhCH2OH instead of (CH2OH)2 was formed 14-50% 2-acetoxymercuri-5-carbethoxy-2,3-dihydrobenzofuran, m. 114-16°

IT 110378-52-4
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 110378-52-4 HCAPLUS

CN Hexamethylenimine, 1-(6-amino-4-pyrimidinyl)- (6CI) (CA INDEX NAME)



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     FILE 'HCAPLUS' ENTERED AT 13:09:18 ON 20 FEB 2008
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L6          2301 SEA FILE=REGISTRY SUB=L5 SSS FUL L4
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L7          1368 L6 AND L3
L8            20 L6 AND C21H35N5
L9            12 L8 AND NC6/ES AND C6/ES AND NCNC3/ES
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